ON LINEAR PROGRAMS WITH LINEAR COMPLEMENTARITY CONSTRAINTS

By

Jing Hu

A Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the Degree of

DOCTOR OF PHILOSOPHY

Major Subject: Mathematical Sciences

Approved by the
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Rensselaer Polytechnic Institute
Troy, New York

September 2008
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ABSTRACT

This thesis concentrates on the studies of linear programs with linear complementarity constraints (LPCCs), and one of the LPCCs' important applications: quadratic programs (QPs). It consists of several fairly independent chapters that address different questions arising in theories and applications of the LPCCs.

In Chapter 1, we give an introduction of the problems that will be studied in this thesis, including the mathematical formulations of the LPCC and the QP, and a review of the existing computational methods for these two problems.

Chapter 2 discusses the different applications of the LPCCs arising from science and engineering. This discussion is not exhaustive, which we believe still sheds some light on the importance of studying the LPCCs.

Chapter 3 presents a parameter-free integer-programming based algorithm for the global resolution of an LPCC. The cornerstone of this approach is to reformulate the LPCC as a minimax integer program, which can then be resolved by applying the Benders decomposition to the inner problem. The algorithm is tested on randomly generated problems with the results attached at the end of this chapter.

Chapter 4 focuses on the topic of indefinite quadratic programming, which have been extensively studied in mathematical programming. The contribution of this thesis is to fill a gap in the existing work on this topic by showing that the global resolution of a feasible QP, which is not known a priori to be bounded or unbounded below, can be accomplished in finite time by solving two LPCCs: the first one confirms whether or not the QP has unbounded objective value on its feasible region; the second LPCC computes the optimal solution if such a solution exists.

As a concluding remark, Chapter 5 provides a summary over the work that has been done in this thesis with some comments on the directions that the future work may possibly lead to.

CHAPTER 1
INTRODUCTION

Linear programs with linear complementarity constraints (LPCCs) are disjunctive linear optimization problems that contain a set of linear complementarity constraints. Mathematical programs with equilibrium constraints (MPECs) can be viewed as a generalization of LPCCs with nonlinear objective functions and nonlinear complementarity constraints. Thus, we will start with an introduction of MPECs in Section 1.1 and present the mathematical formulation of a general LPCC. In addition, we will briefly review some widely accepted algorithms designed for solving MPECs (hence can also be used to solve LPCCs). All such algorithms for solving MPECs, however, can at best compute a stationary solution of some sort. Unlike these methods, our emphasis in this dissertation is the global resolution of the LPCC. The existing methods for globally resolving LPCCs, which require implementing a parameter and computing this parameter in advance, can only be applied to the LPCCs that attain finite optima. This drawback, however, can be avoided in our approach by formulating the LPCC as a parameter-free mixed-integer program. Section 1.2 will mainly focus on the topic of indefinite quadratic programming (QP), which has been extensively studied in mathematical programming. An extensive literature exists pertaining to this topic and will be briefly reviewed in this section. The drawbacks of the existing methods for solving indefinite QPs will also be discussed here.

1.1 Linear Programs with Linear Complementarity Constraints

A mathematical program with equilibrium constraints is an optimization problem that contains two sets of constraints. The first set of constraints are normal functional constraints commonly occurring in general nonlinear programming. The remaining constraints are defined by a set of variational inequalities. Accordingly, the variables can be divided into two sets: $y \in \Re^m$ as the primary variables of the variational inequalities which are parameterized by the rest of the variables $x \in \Re^n$. More specifically, an MPEC can be defined as follows. Suppose that $f : \Re^n \times \Re^m \to \Re$ is the overall objective function to be minimized, $G : \Re^n \times \Re^m \to \Re^l$ defines the functional constraints, and

$F : \Re^n \times \Re^m \to \Re^m$ is the function of the equilibrium. Let $C(x)$ denote the restriction of the variable y for each given x. The variational inequalities that define the equilibrium constraints can be written as:

$$(v - y)^T F(x, y) \geq 0, \quad \forall\, v \in C(x). \tag{1.1}$$

Let $\mathcal{S}(x)$ denote that solution set of the above variational inequalities that are parameterized by x. The MPEC can be formulated as:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & f(x, y) \\ \text{subject to} & G(x, y) \leq 0 \\ \text{and} & y \in \mathcal{S}(x). \end{array}$$

An important special case of the defined variational inequalities (1.1) is when $C(x)$ is equal to $\Re^m_+$. In this case, we can prove that the variational inequalities (1.1) are equivalent to the following complementary conditions:

$$0 \leq y \perp F(x, y) \geq 0.$$

The sign $\perp$ represents that $y^T F(x, y) = 0$, and the above conditions form a standard nonlinear complementarity problem (NCP).

When the function $F(x, y)$ contained in the NCP is linear, say $F(x, y) = Nx + My + q$, the variational inequalities become an LCP (linear complementarity problem), which is parameterized by x. Especially, the following mathematical program:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & c^T x + d^T y \\ \text{subject to} & Ax + By \geq f \\ \text{and} & 0 \leq y \perp w \equiv q + Nx + My \geq 0, \end{array} \tag{1.2}$$

which was historically called a *complementary program* in [37] and an LPEC in [55], is studied in this thesis as a *linear program with linear complementarity constraints* (LPCC).

This complementary problem is also a special instance of disjunctive programming

[7], which defines an optimization problem with disjunctive constraints, by noting that the nonnegativity and complementarity constraints, i.e., $y \geq 0,\, w \geq 0\, y^T w = 0$, are equivalent to

$$y \geq 0,\, w \geq 0 \quad \forall i\ y_i = 0 \text{ or } w_i = 0.$$

The origin of MPECs can be traced back to the economic notion of a Stackelberg game [72], which will be explained in detail in Section 2.4. Another large subclass of MPECs, known as bilevel programs, were introduced in a series of papers by Bracken and McGill [11, 12, 13, 14, 15]. Especially, the bilevel linear/quadratic programs [20], can be formulated as LPCCs; each case has been demonstrated with an example in Section 2.2.

It is well known that typical nonlinear programming (NLP) constraint qualifications do not hold at any feasible solution of an MPEC. This has imposed difficulties to existing NLP solvers. To study an optimal solution of an MPEC, various stationarity concepts have been proposed [22, 27, 52, 60, 58, 63, 70, 80, 81, 82]. Accordingly, many algorithms have been developed to compute stationary solutions of MPECs. These methods generally follow two main approaches: regularization and decomposition.

The basic idea of regularization method is to solve a sequence of nonlinear problems obtained by relaxing the MPEC with a regularization parameter. For instance, the complementary condition $0 \leq y \perp w \geq 0$ can be relaxed with a parameter ρ, which results in a set of nonlinear constraints: $(y, w) \geq 0\ \ y^T w \leq \rho$ [71]. The obtained problem with the relaxed complementarities can be solved applying interior-point methods [50, 65]. An alternative regularization method is based on exact-penalty technique by moving the complementarities in the form of the ℓ_1-norm: $\pi y^T w$ into the objective function, where π is set to be the penalty parameter [47]. Other regularization methods have been proposed to explore different relaxations, including an elastic model [1, 2], smoothing schemes [28, 41], and other approaches [36, 48].

Another approach is a decomposition method which is essentially an extension of pivoting algorithms for solving the linear complementarity problems. This method studies the disjunctive structure of the complementary condition by specifying two index sets for which the two sides of the complementarity constraints are restricted to be 0. It has been shown in [18, 29], that these methods guarantee convergence to stationary solutions under certain assumptions.

An interesting attempt for solving MPECs is to replace the complementarity constraints $0 \leq y \perp w \geq 0$ with a set of nonlinear constraints $(y, w) \geq 0 \;\; y^T w \leq 0$ and apply state-of-the-art NLP solvers directly to the obtained problems. Particularly, the FILTER solver [25], which is available at http://www-neos.mcs.anl.gov/neos/solvers/index.html, has proven to be a very efficient algorithm for computing a solution to the LPCCs in the computational results presented in Section 3.5.

These methods introduced so far are all capable of producing a solution of some sort to the LPCC (1.2); yet they are incapable of ascertaining the quality of the computed solution. This is the major deficiency of these numerical solvers; the primary goal of this thesis is to address this deficiency.

The global resolution of an LPCC has been under investigation in the early work of Ibaraki [37, 38] and Jeroslow [39], who developed cutting-plane methods for solving a so-called *complementarity program*, which is a historical, but not widely used name of LPCC. Recent studies on globally solving LPCCs derived from bilevel programs have been focused on the mixed-integer reformulation and the integer programming methods developed accordingly [4, 5, 33]. There are also several global optimization based methods [30, 31, 73, 77] that are applicable to the LPCCs. Nevertheless, these methods have all preassumed that the given LPCC has a finite optimal objective value. Besides this limitation, computing the value of the parameter "big-M" in the mixed-integer reformulation could be problematic. In Chapter 3, we will present a parameter-free method resolving a given LPCC in finite time, that is the algorithm will terminate with one of the following three mutually exclusive conclusions: the LPCC is infeasible, the LPCC is feasible but has an unbounded objective, or the LPCC attains a finite optimal solution. we will show that the existence of the parameter "big-M" is only conceptual in the mixed-integer formulation whose practical solution does not require the knowledge of the scalar M. To benchmark our algorithm, the general-purposed NLP solvers FILTER and KNITRO will be used in the numerical experiments to solve the class of problems which are guaranteed to be optimally solvable. In addition, we have applied a linear programming based cutting-method as the pre-processor for our algorithm.

1.2 Quadratic Programming

Quadratic programming is among the most important subjects studied in the field of global optimization. It plays a central role in all aspects of mathematical programming. Many real world problems are naturally expressed as quadratic models, such as planning and scheduling, facility allocation and location problems, problems in engineering design and some problems in microeconomics. Such problems can be formulated as quadratic programs (QP) with a quadratic objective function and a set of linear equality or inequality constraints. A general QP can be written as:

$$\begin{aligned} \underset{x\in\Re^n}{\text{minimize}} \quad & q(x) \;\equiv\; \tfrac{1}{2}\, x^T Q x + c^T x \\ \text{subject to} \quad & Ax \;\leq\; b, \end{aligned} \tag{1.3}$$

where c is a vector in $\Re^n$, b is a vector in $\Re^m$, A is a matrix in $\Re^{m\times n}$ and Q is a matrix in $\Re^{n\times n}$. Without any loss of generality, we can assume that matrix Q is symmetric. If this is not the case, we can replace Q with $(Q + Q^T)/2$ and the objective function will remain the same. We will naturally assume that $\{x : Ax \leq b\}$ is a feasible set since the feasibility can be checked by solving a standard linear program. It is well-known that if the matrix Q is positive semidefinite, the problem (1.3) becomes a convex problem, for which any local optimum is globally optimal. In particular, it has been shown that convex quadratic programs can be solved in polynomial time [45]. Nevertheless, a challenging case of the QP is when Q is <u>not</u> positive semidefinite, which is referred to as an indefinite QP.

There is an extensive list of literature on the subject of globally resolving indefinite quadratic programs, particularly on the QPs with simple lower and upper bounds. These QPs with the constraint set as $l \leq x \leq u$, are called box-constrained QPs in some literature. The reference [6] provides an excellent overview of these studies, summarizing the fundamental properties of an indefinite QP, and describing some of the successfully implemented algorithms for subclasses of QPs, such as box-constrained QPs. Yet all these studies have invariably preassumed that the to-be-solved QP attains a finite optimal solution. Hence, a study on the QP which has an unbounded objective value on its feasible region, certainly fills the gap in the existing literature on indefinite QPs, wherein the boundedness of the feasible set has been an essential assumption. One exception is the paper [3], in which the authors developed an algorithm for solving a special class of QP: bilinear program, by reducing the unbounded case to the bounded case via some auxiliary problems with bounded regions. Another noteworthy point is that the existing iterative descent methods for computing stationary solutions require the objective value of the QP to be bounded below (for minimization) on its feasible region. Also, these methods can not be used to test the existence or non-existence of a stationary point in finite time. Nevertheless, the remaining question that is not answered so far in the existing vast amount of literature is: for a given QP, could we come up with a finite method, without any preassumption, to determine whether or not the objective is bounded below (for minimization) or above (for maximization) on its feasible set. In this thesis, we will provide a constructive answer to this question.

It has been proved by Giannessi and Tomasin [32] that if the QP is known to have a finite optimal solution, then the global resolution to this QP can be obtained by finding the stationary point that yields the least objective value. The stationary points of the QP are required to satisfy the first order Karush-Kuhn-Tucker (KKT) conditions, which turn out to be a set of linear complementarity constraints. The quadratic objective of the QP is equivalent to a linear function on the set of stationary points. As a result, a feasible QP, which is known to attain a finite optimal solution, can be reformulated as a new problem of optimizing a linear objective function over the set of the stationary points. This is the well-known LPCC approach for resolving indefinite QPs. About this approach, the papers [16, 17, 78, 79] have proposed algorithms with high efficiency for solving QPs with bounded regions, in particular, box-constrained QPs. With a thorough study on the class of LPCCs to be presented in Chapter 3, one question is raised: is the LPCC approach applicable to a general quadratic program that is not known in advance to have a finite optimal solution? In Chapter 4, we will show how a method can be constructed to effectively determine in finite time if a feasible QP is: unbounded or optimally solvable, with each such outcome being supported by a valid certificate. To validate our approach, we apply the approach to a special class of QPs with just nonnegativity constraints, which are formed to have unbounded objective values. In addition, we will also apply the algorithm to resolve the box-constrained QPs in the form of its equivalent LPCC, and compare the obtained results with the most recent studies on this subject in [79]. At last, a special class of indefinite QPs are formed as an extension of the box-constrained QPs in order to prove at some degree that our algorithm is also applicable to QPs with general linear constraints. Computational results will be presented and discussed in Section 4.5.

CHAPTER 2
THE LPCC AND ITS APPLICATIONS

This chapter gives a short review of the problems arising from science and engineering, that can be formulated as LPCCs via mathematical modelling. Section 2.1 offers a discussion on a special LPCC that arises from financial risk analysis. This is followed by the discussion of two large subclasses of LPCCs. The first one is the class of bilevel programs that is an optimization problem containing another optimization problem in the constraint set; such bilevel programs will be introduced in Section 2.2. The other subclass of LPCCs which contains a set of equilibrium constraints will be discussed in Section 2.4. Section 2.3 addresses an application of the LPCCs pertaining to the MPECs. Section 2.5 provides another application of LPCCs that receives considerable attention in signal processing and image processing. For each application, we desribe the problem briefly, state the defining equations of the model, and give functional expressions for the LPCCs. There is another important application on quadratic programming, which is omitted in this chapter and will be discussed in detail in Chapter 4.

2.1 The Value-At-Risk Minimization Problem in Portfolio Selection

In finance, value-at-risk (VaR) is an estimate of the maximum potential loss with a given confidence level, over a standardized period of time. VaR is one of the most widely accepted and extensively used risk measurements in portfolio selection and financial risk analysis. Despite its popularity, there have been criticisms over the computational difficulties associated with the VaR minimization problem due to its undesirable mathematical characteristics, such as the lack of convexity. Aiming at this difficulty, conditional value-at-risk (CVaR) has been studied as an alternative risk measurement by Rockafellar and Uryasev in [66, 67], in which it has been shown that portfolios with low CVaR will generate a low value of VaR as well. There has been a substantial study about the VaR and CVaR minimization problems. Part of the literature relevant to optimization is as follows, [44, 49, 61, 62, 68, 69, 74]. In particular, [66] focuses on CVaR minimization problems. The global optimal solution of VaR minimization problem has been studied in [64]. In this paper, the VaR problem was first formulated as an instance of LPCC, then resolved by mixed integer programming.

We start by explaining the notations used in the mathematical formulations. Suppose there are n available financial instruments in the portfolio. We use a deterministic vector $x \in \Re^n$ to denote the variable investment, and a closed convex set $X \subset \Re^n$ to denote the collection of feasible investments, such that $x \in X$. Let y be an n-dimensional vector, whose components represent the random losses of the respective financial instruments. For a given vector $x \in X$, $x^T y$ is therefore the random loss associated with the investment. The CVaR, also known as Mean Excess Loss or Mean Shortfall, concerns the average loss that is larger than a certain amount, which is denoted by m. The CVaR associated with an investment x, computes the conditional expected value of losses exceeding m, i.e., it is the mean value of the worst $(1-\beta) * 100\%$ losses, where $\beta \in (0,\, 1)$ denotes the prescribed confidence level of risk. More specifically, the value of CVaR with respect to a given vector x can be computed from the following deterministic quantity [66]:

$$\text{CVaR}_\beta(x) \;\; \equiv \;\; \min_{m \in \Re} \left[m + \frac{1}{1-\beta} \, \mathbb{E}_y \left(x^T y - m \right)_+ \right].$$

In the definition of $\text{CVaR}_\beta(x)$, the notation $\mathbb{E}_y$ represents the expectation with respect to the random vector y; the subscript plus sign denotes the nonnegative part of a scalar (i.e., $t_+ \equiv \max(0,\, t)$). By definition, $\text{CVaR}_\beta(x)$ is computed as the optimal objective value of a linear program parameterized by vector x. Let $\mathcal{M}_\beta$ be the set of minimizers obtained from this linear program. The value of VaR with respect to x is equal to the minimum value among these minimizers, i.e.,

$$\text{VaR}_\beta(x) \;\; \equiv \;\; \min \left\{ m \, : \, m \in \mathcal{M}_\beta(x) \right\}.$$

By comparing the objectives of $\text{VaR}_\beta(x)$ and $\text{CVaR}_\beta(x)$, we have the following result:

$$\text{CVaR}_\beta(x) \; = \; \text{VaR}_\beta(x) + \frac{1}{1-\beta} \, \mathbb{E}_y \left(x^T y \, - \, \text{VaR}_\beta(x) \right)_+ \; \geq \; \text{VaR}_\beta(x).$$

With respect to an investment vector x, $\text{VaR}_\beta(x)$ of a portfolio is the smallest amount m such that, with probability β, the loss will not exceed m, whereas $\text{CVaR}_\beta(x)$ is the conditional expectation of losses above that amount m. The CVaR and VaR minimization problems are, respectively, to choose an investment x such that these two values are minimized over the feasible set X, and they are formulated as follows.

$$\left\{ \begin{array}{ll} \text{minimize} & \text{CVaR}_\beta(x) \\ \text{subject to} & x \in X \end{array} \right\} \text{ and } \left\{ \begin{array}{ll} \text{minimize} & \text{VaR}_\beta(x) \\ \text{subject to} & x \in X \end{array} \right\}.$$

Clearly, the CVaR can be cast equivalently as the following problem in the joint variable (x, m):

$$\begin{array}{ll} \underset{(x,m)\in\Re^{n+1}}{\text{minimize}} & m + \dfrac{1}{1-\beta}\,\mathbb{E}_y\,(x^T y - m)_+ \\ \text{subject to} & x \in X. \end{array}$$

However, the VaR minimization problem can't be formulated as a convex program, due to the fact that the objective $\text{VaR}_\beta(x)$ is not a convex function in the variable x. This is the well-known drawback of using VaR as the risk measurement in portfolio selection.

We assume that the feasible region of investment X is a compact polyhedral, i.e.,

$$X \equiv \{x : Ax \geq b\}.$$

A scenario approach is adopted to discretize the random vector y. Let $\{y^1, y^2, \ldots y^k\}$ be the finite set of scenario values of y. Denote $\{p_1, p_2, \ldots p_k\}$ as the probabilities associated with each scenario, which, summing to one, are assumed to be positive. With this approach, the expectation value with respect to the random vector y becomes:

$$\mathbb{E}_y\,(x^T y - m)_+ = \sum_{i=1}^{k} p_i (x^T y^i - m)_+.$$

Slack variables $\{\tau_i\}_{i=1}^k$, which represent the nonnegative part of $\left\{x^T y^i - m\right\}_{i=1}^k$ respectively, must satisfy the following inequalities:

$$\left\{ \begin{array}{lll} \tau_i & \geq & 0 \\ \tau_i & \geq & x^T y^i - m \end{array} \right\} \quad \forall i = 1 \ldots k.$$

The obtained CVaR minimization problem under the scenario approach is a linear program (LP) in the variable $(m, x, \tau) \in \Re^{1+n+k}$, i.e.,

$$
\begin{aligned}
&\underset{m,x,\tau}{\text{minimize}} && m + \frac{1}{1-\beta}\sum_{i=1}^{k} p_i \tau_i \\
&\text{subject to} && Ax \geq b \\
&\text{and} && \left\{ \begin{array}{lcl} \tau_i & \geq & 0 \\ \tau_i & \geq & x^T y^i - m \end{array} \right\} \quad \forall i = 1 \ldots k.
\end{aligned}
$$

Accordingly, for a given vector $x \in X$, $\text{CVaR}_\beta(x)$ can also be formulated as a linear program in the variable $(m, \tau) \in \Re^{1+k}$.

$$
\begin{aligned}
&\underset{m,\tau}{\text{minimize}} && m + \frac{1}{1-\beta}\sum_{i=1}^{k} p_i \tau_i \\
&\text{subject to} && \left\{ \begin{array}{lcl} \tau_i & \geq & 0 \\ \tau_i & \geq & x^T y^i - m \end{array} \right\} \quad \forall i = 1 \ldots k.
\end{aligned}
\tag{2.1}
$$

By definition, we know that the optimal solutions obtained from the above LP forms the feasible set of the $\text{VaR}_\beta(x)$ problem, which makes the VaR minimization problem a bilevel linear program. The typical approach to resolve such a bilevel linear program is to identify the optimality conditions of the inner problem, leading to linear complementarity constraints, and reformulate the overall problem as an instance of LPCC.

By letting λ_i be the dual variable of the ith functional constraint in (2.1). The optimality conditions of (2.1) are:

$$
\begin{aligned}
&\left\{ \begin{array}{lllll} 0 \leq \tau_i & \perp & \dfrac{p_i}{1-\beta} - \lambda_i & \geq & 0 \\ 0 \leq \lambda_i & \perp & s_i \equiv m + \tau_i - x^T y^i & \geq & 0 \end{array} \right\} \quad \forall i = 1, \ldots, k \\
&\text{and} \quad \sum_{i=1}^{k} \lambda_i = 1,
\end{aligned}
$$

where the $\perp$ denotes the well-known complementarity slackness condition. By collecting the above conditions, the VaR minimization problem can be formulated as an instance of

LPCC in the variables (m, x, τ, λ):

$$
\begin{array}{ll}
\underset{m,x,\tau,\lambda}{\text{minimize}} & m \\
\text{subject to} & Ax \geq b \\
& \left. \left\{ \begin{array}{lllll} 0 \leq \tau_i & \perp & \dfrac{p_i}{1-\beta} - \lambda_i & \geq & 0 \\ 0 \leq \lambda_i & \perp & s_i \equiv m + \tau_i - x^T y^i & \geq & 0 \end{array} \right. \right\} \; \forall i = 1, \ldots, k \\
\text{and} & \displaystyle\sum_{i=1}^{k} \lambda_i = 1,
\end{array}
\tag{2.2}
$$

When selecting an investment in the portfolio, transaction costs should be considered as an important factor. We assume that we have a current portfolio $\bar{x}$, which we wish to modify and obtain a new investment x, such that the transaction costs are minimized. The transaction costs incurred in such a rebalancing is stated as:

$$
f(x) = \sum_{j=1}^{n} \left[g_j \delta(|x_j - \bar{x}_j|) + h_j |x_j - \bar{x}_j| \right],
$$

where g and h are nonnegative vectors and the function $\delta(\cdot)$ is the step function:

$$
\delta(v) = \begin{cases} 1 & \text{if } v > 0 \\ 0 & \text{otherwise.} \end{cases}
$$

$\delta(\cdot)$ is obviously not a continuous function. To deal with this function, we introduce binary variables $y \in \{0, 1\}^n$ to denote $\{\delta(|x_j - \bar{x}_j|)\}_{j=1}^n$, and write the subtraction $x_j - \bar{x}_j$ as the difference between two nonnegative slack variables u_j^+ and u_j^-. The function of the transaction costs becomes:

$$
f(x) = \sum_{j=1}^{n} \left[g_j y_j + h_j (u_j^+ + u_j^-) \right],
$$

under the conditions that

$$
\begin{aligned}
x - \bar{x} &= u^+ - u^- \\
\sigma y &\geq u^+ + u^-.
\end{aligned}
$$

σ is a positive parameter which can be derived by maximizing the ℓ_∞-norm of $x - \bar{x}$ subject to $x \in X$.

The objective of problem (2.2) is modified with a given rebalancing parameter $\rho > 0$, which can be varied in order to trace out a frontier as the desired balance between VaR and the transaction costs varies. The overall problem is formulated as:

$$
\begin{array}{ll}
\underset{m,x,\tau,\lambda,u^{\pm},y}{\text{minimize}} & m \,+\, \rho \displaystyle\sum_{j=1}^{n} \left[\, g_j y_j + h_j(u_j^+ + u_j^-) \,\right] \\
\text{subject to} & Ax \,\geq\, b \\
& \left\{ \begin{array}{lllll} 0 \,\leq\, \tau_i & \perp & \dfrac{p_i}{1-\beta} - \lambda_i & \geq & 0 \\ 0 \,\leq\, \lambda_i & \perp & s_i \,\equiv\, m + \tau_i - x^T y^i & \geq & 0 \end{array} \right\} \;\forall i \,=\, 1, \ldots, k \\
& \displaystyle\sum_{i=1}^{k} \lambda_i \,=\, 1 \\
& \sigma y \,\geq\, u^+ + u^- \\
& 0 \,=\, x - \bar{x} - u^+ + u^- \\
& u^{\pm} \geq 0 \\
& y \in \{0,1\}^n,
\end{array}
\tag{2.3}
$$

2.2 Bilevel Programming

As early as the 1950s, mathematicians have been confronted with an optimization problem, whose constraint set includes another optimization problem. This is nowadays known as a bilevel program, which concerns the optimization problems with multiple decision makers. These decision makers are ordered in a two-layer hierarchical structure, in which the decision maker at a higher hierarchy will strongly influence the decision-making process at the lower hierarchy. This hierarchical relationship reflects the major feature of bilevel programs: they include two mathematical programs within one single framework, the feasible set of one program being a subset of the optimal solution set of the other one. Within such a framework, the former problem is called the *upper-level problem* while the latter one is called to the *lower-level problem*. The optimal solutions of the lower-level problem, which may or may not need to satisfy extra linear or nonlinear constraints, form the feasible set of the upper-level problem. The general formulation of a bilevel program can be stated as:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & F(x,y) \\ \text{subject to} & G(x,y) \leq 0 \\ \text{and} & y \in \underset{y}{\text{argmin}} \{ f(x,y), \ \text{ s.t. } g(x,y) \leq 0 \} \,. \end{array}$$

Corresponding to such a hierarchical structure, the variables are divided into two classes, namely the upper-level variables $x \in \Re^{n_1}$ and the lower-level variables $y \in \Re^{n_2}$. Similarly, the functions $F : \Re^{n_1} \times \Re^{n_2} \to \Re$ and $f : \Re^{n_1} \times \Re^{n_2} \to \Re$ are the upper-level and lower-level objective functions respectively, while the vector functions $G : \Re^{n_1} \times \Re^{n_2} \to \Re^{m_1}$ and $g : \Re^{n_1} \times \Re^{n_2} \to \Re^{m_2}$ define the upper-level and lower-level constraints respectively. It follows that the VaR minimization problem presented in Section 2.1 is a bilevel program, since the $\text{CVaR}_\beta(x)$ is part of the constraint set of the VaR problem. Real-world problems which contain such a two-level hierarchical relationship between the decision makers, arise from many industrial areas, such as revenue management, financial risk analysis, economic planning, chemistry, environmental sciences, optimal control, etc. A review of these detailed applications and general methods for solving these problems can be found in the book [20] and the monograph [76].

The difficulty associated with the bilevel programs lies in the presence of the lower-level problem within the constraint set. Nevertheless, when the lower-level optimization problem is a convex program, the optimal solution set of this problem can be replaced with a system of variational inequalities. This leads to a reformulation of the bilevel program as a mathematical program with equilibrium constraints (MPEC). In this thesis, we focus on the bilevel problems that can be reformulated as LPCCs. One such case is when all the involved functions are affine and the constraints are linear, the obtained problem is a so-called *linear bilevel* program. The other case is when the lower-level problem is a convex quadratic program in the lower-level variables and the upper-level problem is linear program except for the presence of the lower-level problem. We refer this problem as a *linear-quadratic bilevel* program. For each of these two programs, an example will be given to illustrate how to formulate them as LPCCs.

2.2.1 Inverse linear optimization

A typical optimization problem is to determine an optimal decision (optimal solution) provided that the parameters (cost coefficients, right-hand side vector) of the problem are already known. Such problems are defined as forward problems. Conversely, an inverse problem is to estimate the values of the model parameters (cost coefficients, right-hand side vector) based on the values of the decision variables that may be available from historical data, experimental values, or practical observations. Inverse problems are typically encountered when a model or system is being validated. The task is to predict the values of the model's parameters based on the observed outputs of this model. Such applications arise from many areas, including geophysical sciences, facility allocation, network design, portfolio optimization, etc. Inverse linear programming is a special case when the forward problem is a linear program and the task is to identify the parameters of this linear program, including the right-hand side vector of the constraints and the cost coefficients of the objective.

To begin, we assume that the linear program is defined as follows. The decision variable $x \in \Re^n$ is an element of a feasible polyhedral: $\{x : \ Ax = b, \, x \geq 0\}$, where $A \in \Re^{m \times n}$ and $b \in \Re^m$. The cost coefficient vector is denoted as $c \in \Re^n$. Hence, the forward problem is:

$$\begin{aligned} \underset{x \in \Re^n}{\text{minimize}} \quad & c^T x \\ \text{subject to} \quad & Ax = b \\ & x \geq 0. \end{aligned} \tag{2.4}$$

Let $y \in \Re^m$ be the dual variable associated with the constraints $Ax = b$ in (2.4). The dual problem of the linear program (2.4) is formulated as:

$$\begin{aligned} \underset{y \in \Re^m}{\text{maximize}} \quad & b^T y \\ \text{subject to} \quad & A^T y \leq c. \end{aligned}$$

The above problem (2.4) can be solved by identifying a pair of $(x, \, y) \in \Re^{n+m}$, such that the following conditions are satisfied:

$$\begin{aligned} 0 \,\leq\, c - A^T y \;\perp\; x \,\geq\, 0 \\ Ax \,=\, b. \end{aligned} \tag{2.5}$$

Notice that (2.4) can be treated as a linear program parameterized by vectors b and c. Suppose that the vector $(b, c) \in \Re^{m+n}$ is chosen from a feasible polyhedral denoted as $\{(b, c) \in \Re^{m+n} : \, Bb + Cc \geq f\}$, where $B \in \Re^{k \times m}$ and $C \in \Re^{k \times n}$. For each pair of $(b, c) \in \{(b, c) \in \Re^{m+n} : \, Bb + Cc \geq f\}$, there exists a corresponding set of optimal solutions of the parameterized LP (2.4), provided that this problem is feasible and bounded below on its feasible set. Suppose we have observations denoted as $(x^0, \, b^0, \, c^0)$. The inverse linear program is to perturb the cost vector c^0 to c, the right-hand side vector b^0 to b, the decision vector x^0 to x, such that: x is an optimal solution of the new LP parameterized by b and c; while, at the same time, the amount of perturbation, $||(x, b, c) - (x^0, \, b^0, \, c^0)||_p$ ($||v||_p$ denotes the ℓ_p norm of the vector v), is minimized. The mathematical formulation of the inverse problem is given by:

$$\begin{array}{ll} \underset{(x,b,c)}{\text{minimize}} & ||(x, b, c) - (x^0, \, b^0, \, c^0)||_p \\ \text{subject to} & Bb + Cc \geq f \\ \text{and} & x \,\in\, \underset{x^f \in \Re^n}{\text{argmin}} \left\{ c^T \, x^f, \text{ s.t. } Ax^f = b, \, x^f \geq 0 \right\}. \end{array}$$

Apparently, the above problem is cast as a bilevel program in which the lower-level problem is an LP. By introducing the well-known complementary slackness conditions (2.5), we can reformulate the overall inverse problem as:

$$\begin{array}{ll} \underset{(x,y,b,c)}{\text{minimize}} & ||(x, b, c) - (x^0, \, b^0, \, c^0)||_p \\ \text{subject to} & Bb + Cc \geq f \\ \text{and} & 0 \,\leq\, c - A^T y \;\perp\; x \,\geq\, 0 \\ & Ax \,=\, b. \end{array}$$

The above problem becomes an instance of LPCC, if we pick ℓ_1-norm or ℓ_∞-norm to measure the perturbation cost. In what follows, we will use the ℓ_1-norm in the objective function. The formulation of the problem with an ℓ_∞-norm objective can be obtained accordingly. The overall problem with ℓ_1-norm objective is formulated as:

$$\begin{array}{ll}
\underset{(x,y,b,c,r,s,t)}{\text{minimize}} & \sum_{i=1}^{n} r_i + \sum_{i=1}^{m} s_i + \sum_{i=1}^{n} t_i \\
\text{subject to} & r \geq x - x^0 \\
& r \geq x^0 - x \\
& s \geq b - b^0 \\
& s \geq b^0 - b \\
& t \geq c - c^0 \\
& t \geq c^0 - c \\
& Bb + Cc \geq f \\
& Ax = b \\
& 0 \leq c - A^T y \perp x \geq 0,
\end{array}$$

in which $r \in \Re^n$, $s \in \Re^m$ and $t \in \Re^n$ are introduced as the slack variables. This is an instance of an LPCC.

2.2.2 Cross-validated support vector regression

In Section 2.2.1, an example of linear bilevel programming has been presented. In this section, we will show that the other case with the lower-level problem being a convex quadratic program can also be formulated as an LPCC. The reformulation is illustrated using the cross-validated support vector regression problem as an example. Support vector machine, [19, 75], has been used as a successful statistical learning method. However, the performance of this machine learning method heavily depends on the selection of so called hyper-parameters, which need to be pre-defined before the support vector machine problems are solved. One of the well-known methodologies developed to derive the values of the hyper-parameters is to do a grid search on the space of these parameters and perform cross-validation on the whole set of data, [56]. The drawbacks of the grid search are: firstly it neglects the continuity of the parameters; secondly the inefficiency and expense of such a grid search effectively limit the desirable number of hyper-parameters in the model. These drawbacks, however, can be remedied by formulating the cross-validation as a bilevel problem which has the support vector machine as the lower-level problem and uses the out-of-sample error as the outer objective to validate the selection of the hyper-parameters (see [10]). In what follows, we will focus on the regression case, while the classification problems can be treated in a similar fashion (see [9]).

Let's start by explaining the notations. Suppose we have a data set, denoted as Ω, with a total number of ℓ data points. Each of the data points is denoted as $(x_i, y_i)_{i=1}^{\ell} \in \Re^{n+1}$, where x_i is the feature vector of each data point and y_i is the corresponding observation. The cross-validation is to partition these data points into T disjoint subsets $\{\Omega\}_{t=1}^{T}$, each with cardinality $\mathcal{N}_t \equiv |\Omega_t|$ for $t = 1, \ldots, T$. For each partition, the complement of Ω_t, referred as $\overline{\Omega}_t$, consists of points that are not in Ω_t. For a given data set $\overline{\Omega}_t$, a support vector regression problem is to identify a hyperplane in the n-dimensional space to best-fit the data points in $\overline{\Omega}_t$. Overall, there are T support vector regression problems solved on each of the data sets $\left\{\overline{\Omega}_i\right\}_{i=1}^{T}$, and such a hyperplane obtained from $\overline{\Omega}_t$ can be described by $f(x) = x_i^T w^t + b_t$. The support vector regression forms the lower-level optimization problem, which can be stated as:

$$\underset{(w^t, b_t)}{\text{minimize}} \quad C \sum_{i \in \overline{\Omega}_t} \max(\,|\, x_i^T w^t + b_t - y_i \,| - \varepsilon, 0\,) + \frac{1}{2} \parallel w^t \parallel_2^2,$$

in which $\parallel w^t \parallel_2^2$ represents the square of the second norm of w^t, i.e., $\sum_{i=1}^{n} (w_i^t)^2$. The first part of the objective, which appears to be a piecewise linear function, can be cast as a linear function by introducing slack variables $\{e_i^t\}_{i \in \overline{\Omega}_t}$, i.e.,

$$\underset{w^t, b_t}{\text{minimize}} \quad C \sum_{i \in \overline{\Omega}_t} e_i^t + \frac{1}{2} \parallel w^t \parallel_2^2$$

subject to

$$\left\{ \begin{array}{l} e_i^t \geq x_i^T w^t + b_t - y_i - \varepsilon \\ e_i^t \geq -x_i^T w^t - b_t + y_i - \varepsilon \\ e_i \geq 0 \end{array} \right\} \quad i \in \overline{\Omega}_t. \tag{2.6}$$

The problem (2.6) is the classic support vector regression problem with two hyper-parameters C and ε. Provided that C and ε are pre-defined, the second derivative of the objective function with respect to the variable w^t is obviously an identity matrix, which makes the above problem (2.6) a strictly convex quadratic program. The global optimal solution of such a problem is unique and can be identified by resolving the first-order optimality conditions:

$$\begin{aligned} &\left.\begin{cases} 0 \,\leq\, \eta_i^{t,-} \quad \perp \quad x_i^T w^t + b_t - y_i - \varepsilon + e_i^t \,\geq\, 0 \\ 0 \,\leq\, \eta_i^{t,+} \quad \perp \quad y_i - x_i^T w^t - b_t - \varepsilon + e_i^t \,\geq\, 0 \\ 0 \,\leq\, e_i^t \qquad \perp \quad C - \eta_i^{t,+} - \eta_i^{t,-} \,\geq\, 0 \end{cases}\right\} \quad \forall\, i \,\in\, \overline{\Omega}_t \\ &0 \,=\, \sum_{i \in \overline{\Omega}_t} (\, \eta_i^{t,+} - \eta_i^{t,-} \,) \\ &0 \,=\, w^t + \sum_{i \in \overline{\Omega}_t} (\, \eta_i^{t,+} - \eta_i^{t,-} \,)\, x_i, \end{aligned} \tag{2.7}$$

in which $\left\{ \eta_i^{t,\pm} \right\}_{i \in \overline{\Omega}_t}$ are the dual variables associated with the functional constraints listed in (2.6).

The hyper-parameters C and ε are typically selected based on the value of mean square error or mean absolute deviation measured on the out-of-sample data. We will focus on the latter such that the obtained problem has a linear objective function. The absolute deviation of each data point is given by $|\, x_i^T w^t + b_t - y_i \,|$, provided such a data point belonging to Ω_t. The mean absolute deviation, by definition, is computed by taking the average of the absolute deviations of all the data points. The optimal values of C and ε are obtained by identifying such a pair that yields the least value of the mean absolute deviation. Over all the problem is formulated as follows:

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{t=1}^{T} \frac{1}{T} \sum_{i \in \Omega_t} \frac{1}{\mathcal{N}_t} \,|\, x_i^T w^t + b_t - y_i \,| \\ \text{subject to} & \underline{\varepsilon} \le \varepsilon \le \overline{\varepsilon}, \quad \underline{C} \le C \le \overline{C} \\ & \text{for} \quad t \,=\, 1, \ldots, T, \\ & (w^t, b_t) \in \underset{w,b}{\operatorname{argmin}} \left\{ C \displaystyle\sum_{i \in \overline{\Omega}_t} \max(\,|\, x_i^T w + b - y_i \,| - \varepsilon, 0\,) + \frac{1}{2} \,\|\, w \,\|_2^2 \right\}. \end{array} \tag{2.8}$$

After replacing the lower-level problem with its first-order optimality KKT conditions (2.7), the problem (2.8) becomes:

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{t=1}^{T} \frac{1}{T} \sum_{i \in \Omega_t} \frac{1}{\mathcal{N}_t} \,|\, x_i^T w^t + b_t - y_i \,| \\ \text{subject to} & \underline{\varepsilon} \le \varepsilon \le \overline{\varepsilon}, \quad \underline{C} \le C \le \overline{C} \\ & \text{for} \quad t \,=\, 1, \ldots, T, \\ & \left\{ \begin{array}{l} \left. \begin{array}{lll} 0 \,\le\, \eta_i^{t,-} & \perp & x_i^T w^t + b_t - y_i - \varepsilon + e_i^t \,\ge\, 0 \\ 0 \,\le\, \eta_i^{t,+} & \perp & y_i - x_i^T w^t - b_t - \varepsilon + e_i^t \,\ge\, 0 \\ 0 \,\le\, e_i^t & \perp & C - \eta_i^{t,+} - \eta_i^{t,-} \,\ge\, 0 \end{array} \right\} \quad \forall\, i \,\in\, \overline{\Omega}_t \\ 0 \,=\, \displaystyle\sum_{i \in \overline{\Omega}_t} (\,\eta_i^{t,+} - \eta_i^{t,-}\,) \\ 0 \,=\, w^t + \displaystyle\sum_{i \in \overline{\Omega}_t} (\,\eta_i^{t,+} - \eta_i^{t,-}\,)\, x_i. \end{array} \right. \end{array} \tag{2.9}$$

Notice that the objective in the above problem (2.9) is still a piecewise linear function. Since this is a minimization problem, the objective function can be written as a linear function by bringing in slack variables. The details are omitted here and can be checked in [10].

2.3 B-stationarity of MPCCs

Mathematical programs with equilibrium constraints (MPEC) are extensions of bilevel optimization problems. Generally speaking, MPECs are a class of constrained optimization problems in which the essential constraints are defined by variational inequalities or complementarity systems. We will continue with the notation used in Section 1.1 and write a general MPEC as:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & f(x,y) \\ \text{subject to} & G(x,y) \leq 0 \\ \text{and} & y \in \mathcal{S}(x), \end{array}$$

where $\mathcal{S}(x)$ denotes the solution set of:

$$(v-y)^T F(x,y) \geq 0, \quad \forall\, v \in C(x).$$

In the case when the set $C(x)$ is a closed convex set, the above variational inequalities are equivalent to a set of complementarity constraints. To illustrate this equivalence, we will present a special case when $C(x)$ defines a polyhedral: $\{(x,v) \in \Re^{n+m} : Ax + Bv \geq f\}$, where $A \in \Re^{k\times n}$, $B \in \Re^{k\times m}$, and $f \in \Re^k$. It is known that

$$v^T F(x,y) \geq y^T F(x,y), \quad \forall\, v \in C(x).$$

As a result, y is an optimal solution of the following problem:

$$y \in \underset{v}{\text{argmin}} \left\{ v^T F(x,y),\ \text{s.t.}\, Ax + Bv \geq f \right\}.$$

This is a linear program in the variable v, thus can be solved by applying the linear programming complementary slackness. By introducing λ as the dual variable associated with the constraints in the LP, y must satisfy:

$$\begin{aligned} 0 &= F(x,y) + B^T\lambda \\ 0 &\leq \lambda \perp Ax + Bv - f \geq 0, \end{aligned}$$

in which, the sign $\perp$ defines the well known complementarity condition: $\lambda^T(Ax + Bv - f) = 0$. The obtained problem with the variational inequalities (1.1) replaced by the above complementarity constraints, will become a mathematical program with complementarity constraints (MPCC). In what follows, we restrict our discussion to a special class of MPCCs, where $F(x, y)$ is an affine function. Such a problem can be generally formulated as:

$$\begin{array}{ll} \underset{(x,y,w)\in\Re^{n+2m}}{\text{minimize}} & \theta(x,y,w) \\ \text{subject to} & Ax + By + Cw \geq f \\ & 0 \leq y \perp w \geq 0, \end{array} \tag{2.10}$$

where $x \in \Re^n$, $y \in \Re^m$, $w \in \Re^m$, $A \in \Re^{k\times n}$, $B \in \Re^{k\times m}$, $C \in \Re^{k\times m}$, and $\theta : \Re^{n+2m} \rightarrow \Re$ is a continuously differentiable function.

From the point of view of nonlinear programming, the complementarity constraints are problematic, since usual constraint qualifications such as Mangasarian-Fromovitz constraint qualification (MFCQ) is violated at any feasible point (see [85]). As a result, many novel constraint qualifications have been developed to deal with these complementarity constraints. With the aid of these new constraint qualifications, various stationary concepts have been proposed. There has been a substantial list of literature [24, 51, 59, 60, 70, 80, 83, 84, 86, 87] contributing to the study of stationarity (or first-order optimality) conditions for MPCCs. The paper [70] has provided a comprehensive discussion to clarify these concepts and elucidate their connections. In what follows, we focus on so called 'B-stationarity', whose computation and verification are both related to the LPCC formulation. This stationary condition was firstly introduced in the paper [51] and then studied in depth in the monograph [52]. Among various defined stationary conditions, B-stationarity appears to be the strongest first-order optimality conditions for a local minimizer of an MPCC [52].

In order to formally define the B-stationarity, we need to recall the definition of a tangent cone. Specifically, for a given set $X \subset \Re^n$ and a vector $x \in X$, the tangent cone of X at x, denoted as $\mathcal{T}(x; X)$, is the set consisting of the direction vectors dx for which there exists a sequence of vectors $\{x^\nu\} \subset X$ and positive scalars $\{\tau_\nu\} \subset \Re_{++}$, such that

$$\lim_{\nu \to \infty} \tau_\nu = 0 \text{ and } \lim_{\nu \to \infty} \frac{x^\nu - x}{\tau_\nu} = dx.$$

Suppose that the problem (2.10) has at least one feasible solution; such solutions form a feasible set of (2.10), which is denoted as $\mathcal{F}$. Let $(x^0, y^0, w^0) \in \mathcal{F}$ be a feasible solution. We call (x^0, y^0, w^0) a B-stationary point for (2.10), if for all $(dx, dy, dw) \in \mathcal{T}((x^0, y^0, w^0), \mathcal{F})$,

$$\nabla_x \theta(x^0, y^0, w^0)^T dx + \nabla_y \theta(x^0, y^0, w^0)^T dy + \nabla_w \theta(x^0, y^0, w^0)^T dw \geq 0.$$

Apparently, any local minimizer of the MPCC would satisfy the B-stationary conditions. To establish the B-stationarity of a feasible point (x^0, y^0, w^0) of $\mathcal{F}$, it is important and essential to study the local tangent cone $\mathcal{T}((x^0, y^0, w^0), \mathcal{F})$ obtained at this point. However, due to the combinatorial nature of the complementarity conditions, this tangent cone is generally not a convex cone, but a union of several polyhedral cones. More specifically, when degeneracy exists, i.e., $\exists i,\ y_i^0 \cdot w_i^0 = 0$, the tangent cone at (x^0, y^0, w^0) can not be represented by one set of inequality constraints. As a result, the complexity of the tangent cone $\mathcal{T}((x^0, y^0, w^0), \mathcal{F})$ has brought difficulty both to verification and computation of the B-stationarity.

In particular, we define the following index sets which partition the set $\{1, \ldots, m\}$:

$$\begin{aligned}
\alpha(x^0, y^0, w^0) &\equiv \{i : y_i^0 = 0 < w_i^0\} \\
\beta(x^0, y^0, w^0) &\equiv \{i : y_i^0 > 0 = w_i^0\} \\
\gamma(x^0, y^0, w^0) &\equiv \{i : y_i^0 = 0 = w_i^0\}.
\end{aligned}$$

Let $\mathcal{A}(x^0, y^0, w^0)$ be the index set of the constraints $Ax + By + Cw \geq f$ binding at the solution (x^0, y^0, w^0), i.e.,

$$i \in \mathcal{A}(x^0, y^0, w^0) \Leftrightarrow A_{i\bullet} x^0 + B_{i\bullet} y^0 + C_{i\bullet} w^0 = f,$$

where $A_{i\bullet}$ denotes the i's row of the matrix A; similarly for $B_{i\bullet}$ and $C_{i\bullet}$. The tangent cone of $\mathcal{F}$ at the point (x^0, y^0, w^0) can be represented as:

$$\mathcal{T}((x^0, y^0, w^0), \mathcal{F}) \equiv \left\{ \begin{array}{lll} (dx, dy, dw) \in \Re^{n+2m} : & A_{i\bullet}dx + B_{i\bullet}dy + C_{i\bullet}dw \geq 0, & \forall i \in \mathcal{A}(x^0, y^0, w^0) \\ & dy_i \,=\, 0, & \forall i \in \alpha(x^0, y^0, w^0) \\ & dw_i \,=\, 0, & \forall i \in \beta(x^0, y^0, w^0) \\ & 0 \leq dy_i \perp dw_i \geq 0, & \forall i \in \gamma(x^0, y^0, w^0) \end{array} \right\}.$$

Thus, the verification of B-stationarity of (x^0, y^0, w^0) can be accomplished by solving the following problem:

$$\begin{array}{ll} \underset{(dx,dy,dw)}{\text{minimize}} & \nabla_x\theta(x^0, y^0, w^0)^T dx \,+\, \nabla_y\theta(x^0, y^0, w^0)^T dy \,+\, \nabla_w\theta(x^0, y^0, w^0)^T dw \\ \text{subject to} & \\ & \begin{array}{ll} A_{i\bullet}dx + B_{i\bullet}dy + C_{i\bullet}dw \geq 0, & \forall i \in \mathcal{A}(x^0, y^0, w^0) \\ dy_i \,=\, 0, & \forall i \in \alpha(x^0, y^0, w^0) \\ dw_i \,=\, 0, & \forall i \in \beta(x^0, y^0, w^0) \\ 0 \leq dy_i \perp dw_i \geq 0, & \forall i \in \gamma(x^0, y^0, w^0), \end{array} \end{array} \tag{2.11}$$

which constitutes an instance of an LPCC. Based on the definition of B-stationarity, (x^0, y^0, w^0) is a B-stationary point of the MPCC (2.10) if and only if the the problem (2.11) attains a finite optimal solution at 0.

2.4 Stackelberg Game

The equilibrium, firstly studied as a economic phenomena in the field of game theory, now has broadened its application in many areas, including engineering, physics, chemistry. In mathematical programming, variational inequalities are usually used to model the equilibrium; this leads to another subclass of MPECs which contains the equilibrium as part of its constraints. This class of constrained optimization problems possesses a two-layer hierarchical structure similar to that of bilevel problems, except that the lower-level program is an equilibrium rather than an optimization problem. The upper-level presents the decision-makers whose policies lead to some reaction within a particular market or social entity in which the competition takes place; the lower-level presents the players participating in this competition. As an example, we will describe so-called Stackelberg game [72], which contains the Nash equilibrium [57] as the lower-level system under study.

The Stackelberg game can be considered as an extension of the well-known non-cooperative Nash game, which is described as follows. Suppose we have M players in the game, each of whom has a strategy set $Y_i \subseteq \Re^{m_i}$. Let $\theta_i(y_i, y_{-i})$ be the cost functions of player i, where $-i$ denotes the set $\{1, \ldots, M\} \backslash \{i\}$. Provided that the players except for i have chosen their strategies y^0_{-i}, the objective of player i is to select a strategy $y_i \in Y_i$ such that the cost funtion $\theta_i(y_i, y^0_{-i})$ is minimized. Each player observes the action of the remaining players and adjusts his own action until no player has the incentive to deviate from his strategy y^*_i in the sense that

$$y^*_i \in \underset{y_i}{\operatorname{argmin}} \left\{ \theta_i(y_i, y^*_{-i}) \ : \ y_i \in Y_i \right\} \qquad \forall i = 1, \ldots, M$$

Such a strategy tuple $(y^*_1, \ldots, y^*_M)$ is called a Nash equilibrium. Note that if the strategy set Y_i of each player i is a given closed convex set and the cost function $\theta_i(\cdot, y_{-i})$ is convex and continuous differentiable, the Nash equilibrium can be formulated as a system of variational inequalities. Especially, if Y_i is a polyhedral for each player i and $\theta_i(\cdot)$ is a linear funtion, the Nash equilibrium can be resolved by solving a group of linear complementary conditions.

In contrast, the Stackelberg game has a distinctive player (called the *leader*), who can anticipate the other players' (called the *followers*) reaction and select his optimal strategy accordingly. Corresponding to an arbitrary strategy selected by the leader, the followers select their own optimal strategies and form a Nash equilibrium. More precisely, the leader chooses a strategy x from his strategy set $X \subseteq \Re^n$; corresponding to such a strategy $x \in X$, each of the followers, say i, has a strategy set $Y_i(x) \subseteq \Re^{m_i}$ and the cost function $\theta_i(x, y_i, y_{-i})$. Note that each follower has his strategy set dependent on the leader's strategy and the cost function dependent on both the leader's and the followers' strategies. Based on the Nash non-cooperative principle described above, the followers will choose, for a fixed and arbitrary $x \in X$, a joint response vector

$$y^* \equiv (y_i^*)_{i=1}^M \in \prod_{i=1}^M Y_i(x)$$

such that for each $i = 1, \ldots, M$

$$y_i^* \in \operatorname*{argmin}_{y_i} \left\{ \theta_i(x, y_i, y_{-i}^*) \,:\, y_i \in Y_i(x) \right\}.$$

Assume that, for an arbitrary $x \in X$, the strategy sets $\{Y_i(x)\}_{i=1}^M$ are closed and convex, and the cost functions $\{\theta_i(x, y_i, y_{-i})\}_{i=1}^M$ are convex and continuous differentiable in the variables $\{y_i\}_{i=1}^M$ respectively. It follows that the tuple y^* must satisfy the following variational inequalities:

$$\begin{aligned} &\forall i = 1, \ldots, M \\ &\quad (y_i - y_i^*)^T \nabla_{y_i} \theta_i(x, y_i^*, y_{-i}^*) \geq 0, \ \forall y_i \in Y_i(x) \end{aligned} \tag{2.12}$$

Let $f : \Re^{n+\sum_{i=1}^M m_i} \to \Re$ be the cost function of the leader which depends on both his own and the followers' strategies. The Stackelberg game is therefore to determine a vector $(x, y) \in \Re^{n+\sum_{i=1}^M m_i}$ in order to

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & f(x, y) \\ \text{subject to} & x \in X \\ \text{and} & (2.12) \end{array} \tag{2.13}$$

If we assume that each of the followers' cost functions, say $\theta_i(x, y)$, is linear in the variables (x, y), or linear in (x, y_{-i}) and convex quadratic in y_i, the obtained variational inequalities (2.12) can be rewritten as a group of linear complementary conditions. If we further assume that the cost function of the leader $f(\cdot)$ is a linear function, the obtained problem (2.13) will become an instance of LPCC. Stackelberg game problems have been studied extensively by economists and has found wide application in many areas, including optimal product design, quality control in services, and the pricing of electric transmission. In this thesis, we do not focus a specific problem; instead we give a general framework to illustrate the reformulation of the stackelberg problem as an LPCC.

2.5 The ℓ_0-norm Minimization Problem

Another important application of LPCC can be found in the ℓ_0-norm minimization problem, which is encountered when a solution to an underdetermined system of linear equations is desired with as many of its components equal to zero as possible. For example, in signal processing, a sparse overcomplete representation is more desirable than dense ones, that is, approximating the signal as linear combinations of as few elementary functions from a large dictionary as possible. Thus, ℓ_0-norm minimization problem has received considerable interest in the areas of sparse approximation and signal processing. The main goal of these activities is to ensure the efficient recovery of sparse solutions, i.e., solutions have few nonzero components, to under-determined linear systems $Ax = b$ with $A \in \Re^{m\times n}$, $b \in \Re^m$. The mathematical formulation of this problem can be stated as:

$$\begin{aligned} \underset{x\in\Re^n}{\text{minimize}} \quad & ||x||_0 \\ \text{subject to} \quad & Ax = b, \end{aligned} \tag{2.14}$$

in which the matrices $A \in \Re^{k\times n}$, $B \in \Re^{k\times m}$ and the vector $b \in \Re^k$ are pre-defined. In the objective function of problem (2.14), $||x||_0$ denotes the number of the nonzero components of vector x. Note the linear constraints contained in the formulation could be given in a more general form. Instead we formulate the ℓ_0-norm minimization problem as (2.14), since this the most frequently studied problem in the existing literature.

Some of the existing methods for solving (2.14) are aimed at approximating a solution by minimizing the ℓ_1-norm instead. The obtained problem which is to minimize ℓ_1-norm of x subject to $Ax = b$, can be formulated as a linear program. This approach, entitled *basis pursuit* [21], is apparently a very efficient way to recover a sparse solution of the underdetermined linear system. Unfortunately, the obtained solution by minimizing the ℓ_1-norm generally is not the sparsest solution. Although, basis pursuit can be applied to approximate sparse solutions of linear systems, we are still more interested in minimizing the ℓ_0-norm. One must note that the exact recovery of the sparsest solution is computationally hard, and can be only applied to smaller instances to optimality.

Let's return to the problem (2.14). To count the number of nonzero elements of vector x, a vector ζ with the same dimension as x is brought into the formulation and stated as:

$$\zeta_i = \begin{cases} 0, & \text{if } x_i = 0 \\ 1, & \text{if } x_i \neq 0 \end{cases} \qquad \forall i = 1 \ldots n.$$

Accordingly, the objective function can be written as the sum of the components of ζ, i.e., $||x||_0 = \sum_{i=1}^n \zeta_i$. By writing the vector x as the difference of two nonnegative vectors, i.e., $x = x^+ - x^-$, it is obvious that the vector ζ must satisfy the following linear complementarity conditions:

$$\begin{aligned} 0 \leq x^+ + x^- \quad &\perp \quad 1 - \zeta \geq 0 \\ x = x^+ - x^- \quad & \qquad\;\; \zeta \geq 0. \end{aligned}$$

The obtained LPCC is formulated as:

$$\begin{aligned} \underset{x^\pm, \zeta}{\text{minimize}} \quad & \sum_{i=1}^n \zeta_i \\ \text{subject to} \quad & Ax^+ - Ax^- = b, \\ & 0 \leq x^+ + x^- \perp 1 - \zeta \geq 0 \\ & x^+, x^-, \zeta \geq 0. \end{aligned} \tag{2.15}$$

The equivalence between (2.14) and (2.15) can be recognized by noting the following facts. First of all, given an optimal solution $(x^\pm, \zeta)$ of the problem (2.15), we can construct a vector x feasible to (2.14) by letting $x = x^+ - x^-$. This vector x must be optimal to (2.14) as well. Suppose this is not that case; in other words there exists a solution x' feasible to (2.14) such that $||x||_0 > ||x'||_0$. By letting $x'^+ - x'^- = x'$ and

$$\zeta'_i = \begin{cases} 0, & \text{if } x'_i = 0 \\ 1, & \text{if } x'_i \neq 0 \end{cases} \qquad \forall i = 1 \ldots n,$$

we have $(x'^\pm, \zeta')$ feasible to (2.15) with $\sum_{i=1}^n \zeta'_i < \sum_{i=1}^n \zeta_i$, which leads to a contradiction. Conversely, we can prove in a similar fashion that any optimal solution of (2.14) must be optimal to (2.15).

Another area where the ℓ_0-norm minimization problem arises is in machine learning, or more specifically, to minimize the number of the misclassified data points in a classification problem. The reference [55] has studied in detail how to reformulate the misclassification minimization problems as LPCCs. The classification problem is to identify a hyperplane in n-dimensional real space such that the data points with different labels can be seperated. Suppose we have a finite set of labeled data points, $\{(x_i, y_i)\}_{i=1}^N \subset \Re^{n+1}$. The label y_i takes value from $\{1, -1\}$, where the value 1 indicates the data point i is in one data set, and the value -1 indicates the other case when i is in the other set. The plane, denoted as $f(x) = x_i^T w + b$, has one data set lying on one side and the other data set lying on the other side. The misclassification defines the case that the date point by label y_i should be in one set, but is set to be in the other set by function $f(x)$. The vector ζ in the dimension of N is introduced to count the misclassified points, with each component $i = 1 \ldots N$ stated as:

$$\zeta_i = \begin{cases} 1 & -y_i(x_i^T w + b) > 0 \\ 0 & -y_i(x_i^T w + b) \leq 0. \end{cases}$$

The number of misclassified points, accordingly, can be stated as $\sum_{i=1}^N \zeta_i$. By introducing additional variables z with dimension of N, ζ must satisfy the following linear complementarity conditions:

$$\left.\begin{array}{l} 0 \leq \zeta_i \ \perp \ y_i(x_i^T w + b) + z_i \geq 0 \\ 0 \leq z_i \ \perp \qquad\qquad\quad 1 - \zeta_i \geq 0 \end{array}\right\} \quad \forall\, i = 1 \ldots N.$$

The overall misclassification minimization problem can be formulated as:

$$\begin{array}{ll} \underset{w,b,z,\zeta}{\text{minimize}} & \displaystyle\sum_{i=1}^N \zeta_i \\ \text{subject to} & \\ & \left.\begin{array}{l} 0 \leq \zeta_i \ \perp \ y_i(x_i^T w + b) + z_i \geq 0 \\ 0 \leq z_i \ \perp \qquad\qquad\quad 1 - \zeta_i \geq 0 \end{array}\right\} \quad \forall\, i = 1 \ldots N. \end{array} \tag{2.16}$$

The above problem (2.16) is a simplified classification problem. A more frequently used classification method is to implement so-called cross-validated support vector machine.

The method is similar to the cross-validated support vector regression problem illustrated in Section 2.2.2, excpet that the lower-level problem is a support vector classfication problem instead. The obtained overall problem also turned out to be an instance of LPCC. The details can be found in [9].

CHAPTER 3
GLOBALLY RESOLVING THE LPCCS

In this chapter, we will present a method for globally resolving LPCCs, that is the algorithm is able to identify the infeasibility or unboundedness of an LPCC, or compute the optimal solution if the LPCC is optimally solvable. The proposed method begins with a reformulation of the LPCC as a mixed-integer problem which involves a conceptually very large parameter (denoted as θ). The existence of this parameter is not guaranteed unless the assumption of boundedness holds. After fixing the integer variables, the obtained problem is a standard linear problem (LP). Via dualization of this LP, the parameter θ could be removed, which results in an equivalent formulation of the LPCC as a minmax 0-1 integer program (IP). By applying Benders decomposition [46], the global resolution of this IP can be determined, yielding a certificate for the three states of the LPCC, without any *a priori* boundedness assumption. The implementation of this parameter-free algorithm is accomplished by solving two types of subproblems. The first type is a standard LP and the second type is an IP defined solely by *satisfiability constraints* [8, 40]. Each of these constraints corresponds to a certain *piece* (or several pieces) of the LPCC. The algorithm can be interpreted as searching on the finitely many pieces of the LPCC, with the search guided by solving the satisfiability IPs.

The organization of this chapter is as follows. Section 3.1 summarizes the three states of the LPCC, introduces the minmax IP formulation, and provides a proof of the equivalence between the IP and the original LPCC. Section 3.2 presents how to solve the minmax IP by applying Bender's approach. Key steps of the algorithm, including the implemented pre-processor and the sparsification of the satisfiability constraints, are explained in Section 3.3. The detailed algorithm is presented in Section 3.4, wherein a numerical example has been given. Experiments and computational results will be presented in Section 3.5.

3.1 Preliminary Discussion

Borrowing the notations used in Section 1.1, an LPCC can be generally formulated as:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & c^T x + d^T y \\ \text{subject to} & Ax + By \geq f \\ \text{and} & 0 \leq y \perp q + Nx + My \geq 0, \end{array} \tag{3.1}$$

where the vectors $c \in \Re^n$, $d \in \Re^m$, $f \in \Re^k$, $q \in \Re^m$, and the matrices $A \in \Re^{k\times n}$, $B \in \Re^{k\times m}$, $M \in \Re^{m\times m}$, $N \in \Re^{m\times n}$ are already known. The sign $\perp$ denotes the complementarity condition, i.e., $0 \leq a \perp b \geq 0 \Rightarrow \forall i \in \{1 \ldots |a|\},\ a_i \cdot b_i = 0$. The LPCC is equivalent to the minimization of a finite number of linear programs. Each such linear program is defined as one *piece* of the LPCC. More specifically, with a subset $\alpha \subseteq \{1, \cdots, m\}$ with its complement $\bar{\alpha} \equiv \{i : i = 1 \ldots m, \text{and}\, i \notin \alpha\}$, each piece of the LPCC can be formulated as the following LP(α):

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & c^T x + d^T y \\ \text{subject to} & Ax + By \geq f \\ & (\, q + Nx + My\,)_\alpha \geq 0 = y_\alpha \\ & (\, q + Nx + My\,)_{\bar{\alpha}} = 0 \leq y_{\bar{\alpha}}. \end{array} \tag{3.2}$$

With m complementarity conditions contained in the constraint set of (3.1), the LPCC has 2^m pieces. The following statements reveals the equivalence between the LPCC and the 2^m LP pieces associated with it.

(a) the LPCC (3.1) is infeasible if and only if $\forall\, \alpha \subseteq \{1, \cdots, m\}$, LP($\alpha$) is infeasible ;

(b) the LPCC (3.1) is feasible and has an unbounded objective if and only if $\exists \alpha \subseteq \{1, \cdots, m\}$, such that the LP($\alpha$) is feasible and has an unbounded objective;

(c) the LPCC (3.1) is feasible and attains a finite optimal solution if and only if (i) there exists at least one subset α of $\{1, \cdots, m\}$ such that the LP(α) is feasible, and (ii) every such feasible LP(α) is bounded below on its feasible region. Moreover, the optimal objective value of the LPCC (3.1), denoted LPCC$_{\min}$, is given by the LP(α)

that yields the minimum optimal objective value among all the feasible pieces.

Obviously, the global resolution of the LPCC can be obtained by completely resolving these 2^m LPs. Unfortunately, the proves to a very inefficient computational methodology, since the number of the LPs exponentially grows with the complementarities. Another frequently used approach is based on an "equivalent" IP formulation of (3.1), wherein the complementarity constraint is reformulated in terms of the binary vector $z \in \{0, 1\}^m$ and a conceptually very large scalar $\theta > 0$:

$$\begin{array}{lrcl} \underset{(x,y,z)}{\text{minimize}} & c^T x + d^T y & & \\ \text{subject to} & Ax + By & \geq & f \\ & \theta\, z \,\geq\, q + Nx + My & \geq & 0 \\ & \theta(\,\mathbf{1} - z\,) \,\geq\, y & \geq & 0 \\ \text{and} & z & \in & \{\,0, 1\,\}^m, \end{array} \tag{3.3}$$

where $\mathbf{1}$ is the m-vector of all ones. The value of θ can be computed by solving LPs to obtain bounds on the variables y and the constraints $q+Nx+My$. With a valid value of θ, we can then solve the IP (3.3) by applying various integer programming based techniques. The drawback of this approach is firstly it is only applicable to the LPCCs with bounded feasible regions. Besides this limitation, computing the valid bounds could be difficult even if they are known to exist implicitly. Our approach, in contrast, is able to remove this restriction by eliminating θ from the IP formulation. We start the discussion of this approach by noting that the problem (3.3) can be treated as a linear program parameterized by θ and z.

For a given binary vector z and a positive scalar θ, we denote the following LP as LP(θ, z):

$$\begin{array}{lrcll}
\underset{(x,y)}{\text{minimize}} & c^T x + d^T y & & & \\
\text{subject to} & Ax + By & \geq & f & (\lambda) \\
& Nx + My & \geq & -q & (u^-) \\
& -Nx - My & \geq & q - \theta\, z & (u^+) \\
& -y & \geq & -\theta\,(\mathbf{1} - z) & (v) \\
\text{and} & y & \geq & 0, &
\end{array} \tag{3.4}$$

The variables in the parentheses denote the dual variables associated with each set of the constraints listed at the front. Thus, the dual of (3.4), which we denote as DLP(θ, z), is:

$$\begin{array}{ll}
\underset{(\lambda, u^{\pm}, v)}{\text{maximize}} & f^T \lambda + q^T(u^+ - u^-) - \theta\,\left[\, z^T u^+ + (\mathbf{1} - z)^T v \,\right] \\
\text{subject to} & A^T \lambda - N^T(u^+ - u^-) \,=\, c \\
& B^T \lambda - M^T(u^+ - u^-) - v \,\leq\, d \\
\text{and} & (\lambda, u^{\pm}, v) \,\geq\, 0.
\end{array} \tag{3.5}$$

Let $\Xi \subseteq \Re^{k+3m}$ be the feasible region of DLP(θ, z), i.e.,

$$\Xi \,\equiv\, \left\{ \begin{array}{ll} (\lambda, u^{\pm}, v) \,\geq\, 0 \,: & A^T \lambda - N^T(u^+ - u^-) \,=\, c \\ & B^T \lambda - M^T(u^+ - u^-) - v \,\leq\, d \end{array} \right\}. \tag{3.6}$$

Note that in DLP(θ, z), θ and z have been removed from the constraints into the objective. The feasible region Ξ is a fixed polyhedron independent of the pair (θ, z). Since Ξ is a subset of the nonnegative orthant $\Re^n_+$, this set has at least one extreme point if it is nonempty. Throughout, we will adopt the standard convention that the objective value $-\infty$ (∞) indicates the infeasibility of a maximization (minimization, respectively) problem. We summarize the basic relations between the above programs in the following proposition.

Proposition 1. The following three statements hold.

(a) From any feasible solution (x^0, y^0) of (3.1), we can induces a pair (θ_0, z^0), where θ_0 is a positive scalar and z^0 is a binary vector in $\{0,1\}^m$, such that the tuple (x^0, y^0, z^0) is feasible to (3.3) for all $\theta \geq \theta_0$; such a z^0 has the property that

$$\begin{aligned} (\, q + Nx^0 + My^0 \,)_i \,>\, 0 \;\;&\Rightarrow\;\; z_i^0 \,=\, 1 \\ (\, y^0 \,)_i \,>\, 0 \;\;&\Rightarrow\;\; z_i^0 \,=\, 0. \end{aligned} \tag{3.7}$$

(b) Conversely, if (x^0, y^0, z^0) is a feasible solution of (3.3) for some $\theta \geq 0$, then (x^0, y^0) is feasible to (3.1).

(c) If (x^0, y^0) is an optimal solution to (3.1), then it is optimal to the LP(θ, z^0) for all pairs (θ, z^0) such that $\theta \geq \theta_0$ and z^0 satisfies (3.7); moreover, for each $\theta > \theta_0$, any optimal solution $(\widehat{\lambda}, \widehat{u}^{\pm}, \widehat{v})$ of the DLP(θ, z^0) satisfies $(z^0)^T \widehat{u}^+ + (\, \mathbf{1} - z^0 \,)^T \widehat{v} = 0$.

Proof. The proofs of (a) and (b) are nontrivial and omitted here. We will proceed with the proof of (c). Let (x^0, y^0) denote the optimal solution of (3.1). With a pair (θ, z^0) such that $\theta \geq \theta_0$ and $z^0 \in \{0,1\}^m$ satisfies (3.7), (x^0, y^0) must be feasible to the LP(θ, z^0); hence

$$c^T x^0 + d^T y^0 \;\geq\; \text{LP}_{\min}(\theta, z^0), \tag{3.8}$$

where $\text{LP}_{\min}(\theta, z^0)$ denotes the optimal objective value of LP(θ, z^0). The reverse inequality must hold because of (b) and the optimality of (x^0, y^0) to (3.1). Consequently, equality holds in (3.8). For $\theta > \theta_0$, if i is such that $z_i^0 > 0$, then

$$(\, q + Nx^0 + My^0 \,) \;\leq\; \theta_0 \, z_i^0 \; < \theta \, z_i^0,$$

and complementary slackness implies that $(\widehat{u}^+)_i = 0$. Similarly, we can show that $z_i^0 = 0 \Rightarrow v_i = 0$. Hence (c) follows. $\square$

3.1.1 The parameter-free dual programs

Motivated by Part (c) of Proposition 1, we define the following two value functions on the binary vectors. For any $z \in \{0,1\}^m$, we define

$$\begin{array}{rll} \Re \cup \{\pm\infty\} \ni \varphi(z) \equiv & \underset{(\lambda, u^\pm, v)}{\text{maximum}} & f^T\lambda + q^T(u^+ - u^-) \\ & \text{subject to} & A^T\lambda - N^T(u^+ - u^-) = c \\ & & B^T\lambda - M^T(u^+ - u^-) - v \le d \\ & & (\lambda, u^\pm, v) \ge 0 \\ & \text{and} & z^T u^+ + (\mathbf{1} - z)^T v \le 0 \end{array} \tag{3.9}$$

and its homogenization:

$$\begin{array}{rll} \{0, \infty\} \ni \varphi_0(z) \equiv & \underset{(\lambda, u^\pm, v)}{\text{maximum}} & f^T\lambda + q^T(u^+ - u^-) \\ & \text{subject to} & A^T\lambda - N^T(u^+ - u^-) = 0 \\ & & B^T\lambda - M^T(u^+ - u^-) - v \le 0 \\ & & (\lambda, u^\pm, v) \ge 0 \\ & \text{and} & z^T u^+ + (\mathbf{1} - z)^T v \le 0. \end{array} \tag{3.10}$$

Note that we have placed the equality condition $z^T u^+ + (\mathbf{1} - z)^T v = 0$ as an inequality in the constraint sets of (3.9) and (3.10). This modification is valid since all the involved variables are nonnegative and $z \in \{0,1\}^m$. Apparently, (3.10) is always feasible, and $\varphi_0(z)$ either attains optimality at 0 or is unbounded (valued by ∞). However, the feasibility of (3.9) depends on the pair (c, d); thus $\varphi(z) \in \Re \cup \{\pm\infty\}$. Especially, for any pair (c, d) with which (3.9) is feasible, we have

$$\varphi(z) < \infty \Leftrightarrow \varphi_0(z) = 0.$$

Furthermore, we will illustrate this equivalence in the following proposition that describes a one-to-one correspondence between (3.10) and the feasible pieces of the LPCC. The *support* of a vector z, denoted as $\text{supp}(z)$, defines the index set of the nonzero components of z.

Proposition 2. For any $z \in \{0,1\}^m$, $\varphi_0(z) = 0$ if and only if the LP(α) is feasible, where $\alpha \equiv \text{supp}(z)$.

Proof. By multiplying the last constraint of (3.10) with a scalar $\theta > 0$, we can formulate the dual of (3.10) as

$$\begin{array}{lrcl} \underset{(x,y)}{\text{minimize}} & 0^T x + 0^T y & & \\ \text{subject to} & Ax + By & \geq & f \\ & \theta\, z \;\geq\; q + Nx + My & \geq & 0 \\ \text{and} & \theta\,(\,\mathbf{1} - z\,) \;\geq\; y & \geq & 0. \end{array} \tag{3.11}$$

By LP duality, $\varphi_0(z) = 0$, if and only if its dual problem (3.11) is feasible for some $\theta > 0$. Apparently (3.11) is feasible for some $\theta > 0$ if and only if the LP(α) is feasible for $\alpha \equiv$ supp(z). □

We need to clarify the relation between the extreme points/rays of the feasible region of (3.9) and those of the feasible set Ξ.

Proposition 3. For any $z \in \{0,1\}^m$, given a vector $(\lambda^p, u^{\pm,p}, v^p)$ feasible to (3.9), it is an extreme point in the feasible region of (3.9) if and only if it is extreme in Ξ; given a feasible ray $(\lambda^r, u^{\pm,r}, v^r)$ of (3.9), it is an extreme ray in this region if and only if it is extreme in Ξ.

Proof. We only need to prove the first assertion; the second one can be proved similarly. The sufficiency is obvious. The converse can be proved by controversy. Suppose that $(\lambda^p, u^{\pm,p}, v^p)$ is an extreme solution of (3.9). Then this triple must be an element of Ξ. If it lies on the line segment of two other feasible solutions of Ξ, then the latter two solutions must satisfy the additional constraint $z^T u^+ + (\mathbf{1} - z)^T v \leq 0$. This obviously doesn't hold since we already assumed that $(\lambda^p, u^{\pm,p}, v^p)$ is an extreme solution. Therefore, $(\lambda^p, u^{\pm,p}, v^p)$ is also extreme in Ξ. □

3.1.2 The set $\mathcal{Z}$ and a minimax formulation

Proposition 2 has described an important property of the binary vector $z \in \{0,1\}^m$ that defines one feasible piece of the LPCC (3.1). Based on this property, we can define the key set of binary vectors:

$$\mathcal{Z} \equiv \{ z \in \{0,1\}^m : \varphi_0(z) = 0 \},$$

which is the feasibility descriptor of the feasible pieces of the LPCC (3.1). This definition leads to the following minimax integer program:

$$\underset{z \in \mathcal{Z}}{\text{minimize}}\ \varphi(z) \equiv \left[\begin{array}{ll} \underset{(\lambda, u^{\pm}, v)}{\text{maximum}} & f^T\lambda + q^T(u^+ - u^-) \\ \text{subject to} & A^T\lambda - N^T(u^+ - u^-) = c \\ & B^T\lambda - M^T(u^+ - u^-) - v \leq d \\ & (\lambda, u^{\pm}, v) \geq 0 \\ \text{and} & z^T u^+ + (\mathbf{1} - z)^T v \leq 0. \end{array} \right] \tag{3.12}$$

Note that $\mathcal{Z}$ is a finite set. For any $z \in \mathcal{Z}$, $\varphi_0(z)$ is, by definition, equal to 0. It follows that $\varphi(z) \in \Re \cup \{-\infty\}$. Thus $\underset{z \in \mathcal{Z}}{\text{argmin}}\, \varphi(z) \neq \emptyset$ if and only if $\mathcal{Z} \neq \emptyset$. The following proposition rephrases the three basic facts that connect the LPCC with its LP pieces in terms of the IP (3.12).

Theorem 4. The following three statements hold:

(a) the LPCC (3.1) is infeasible if and only if $\min_{z \in \mathcal{Z}} \varphi(z) = \infty$ (i.e., $\mathcal{Z} = \emptyset$);

(b) the LPCC (3.1) is feasible and has an unbounded objective value if and only if $\min_{z \in \mathcal{Z}} \varphi(z) = -\infty$ (i.e., $z \in \mathcal{Z}$ exists such that $\varphi(z) = -\infty$);

(c) the LPCC (3.1) attains a finite optimal solution if and only if $-\infty < \min_{z \in \mathcal{Z}} \varphi(z) < \infty$.

In all cases, $\text{LPCC}_{\min} = \min_{z \in \mathcal{Z}} \varphi(z)$; moreover, for any $z \in \{0,1\}^m$ for which $\varphi(z) > -\infty$, $\text{LPCC}_{\min} \leq \varphi(z)$.

Proof. Statement (a) immediately holds as a result of Proposition 2. Suppose that the LPCC (3.1) is feasible and has an unbounded objective value. Then an index set $\alpha \subseteq \{1, \cdots, m\}$ exists such that the LP(α) is feasible and unbounded below. By letting $z \in \{0,1\}^m$ be such that $\text{supp}(z) = \alpha$ and $\bar{\alpha}$ be the complement of α in $\{1, \cdots, m\}$, we have

$z \in \mathcal{Z}$. Moreover, the dual of the (unbounded) LP(α) is

$$\begin{array}{lll} \underset{(\lambda, u_{\bar{\alpha}}, u_{\alpha}^-)}{\text{maximize}} & f^T\lambda + (\, q_{\bar{\alpha}}\,)^T u_{\bar{\alpha}} - (\, q_{\alpha}\,)^T u_{\alpha}^- & \\ \text{subject to} & A^T\lambda - (\, N_{\bar{\alpha}\bullet}\,)^T u_{\bar{\alpha}} + (\, N_{\alpha\bullet}\,)^T u_{\alpha}^- \,=\, c & \\ & (\, B_{\bullet\bar{\alpha}}\,)^T\lambda - (\, M_{\bar{\alpha}\bar{\alpha}}\,)^T u_{\bar{\alpha}} + (\, M_{\alpha\bar{\alpha}}\,)^T u_{\alpha}^- \,\leq\, d_{\bar{\alpha}} & \\ \text{and} & (\, \lambda, u_{\alpha}^-\,) \,\geq\, 0, & \end{array} \tag{3.13}$$

in which the $\bullet$ in the subscripts is the standard notation in linear programming, denoting rows/columns of matrices. This problem (3.13) is equivalent to (3.9), since u_{α}^+ and $u_{\bar{\alpha}}^-$ are both 0 in (3.9). By LP duality, (3.13) is infeasible; thus it follows that $\varphi(z) = -\infty$ by convention. Conversely, suppose that $z \in \mathcal{Z}$ exists such that $\varphi(z) = -\infty$. By definition of $\mathcal{Z}$, we know that $\varphi_0(z) = 0$. Let $\alpha \equiv \text{supp}(z)$ and $\bar{\alpha} \equiv$ complement of α in $\{1, \cdots, m\}$. By Proposition 2, the LP(α) must be feasible. Moreover, since $\varphi(z) = -\infty$, it follows that (3.13), being equivalent to (3.9), is infeasible; thus the LP(α) is unbounded. Statement (c) follows readily from (a) and (b). The equality between LPCC$_{\min}$ and $\min\limits_{z \in \mathcal{Z}} \varphi(z)$ is due to the equivalence between (3.13) and (3.9), where the former LP is essentially the dual of the piece LP(α). To prove the last assertion of the theorem, let $z \in \{0,1\}^m$ be such that $\varphi(z) > -\infty$. Without loss of generality, we may assume that $\varphi(z) < \infty$. Thus the LP (3.9) attains a finite maximum; hence $\varphi_0(z) = 0$. Therefore $z \in \mathcal{Z}$ and the bound LPCC$_{\min} \leq \varphi(z)$ holds readily. □

3.2 The Benders Approach

In what follows, we will apply Bender's approach to the mixed IP (3.12), whose resolution is also globally optimal to the LPCC (3.1) according to Proposition 4. Let $\left\{ \left(\lambda^{p,i}, u^{\pm,p,i}, v^{p,i} \right) \right\}_{i=1}^K$ and $\left\{ \left(\lambda^{r,j}, u^{\pm,r,j}, v^{r,j} \right) \right\}_{j=1}^L$ be the set of the extreme points and extreme rays of the feasible set Ξ, respectively. Note that, if Ξ is a feasible set, there is at least one extreme point ($K \geq 1$). The generation of these extreme points and rays will be discussed later in this section. In what follows, we take them as available in order to derive a restatement of Theorem 4 in terms of these extreme points and rays.

By standard Bender's approach, the IP (3.12) can be written as:

$$\underset{z\in\mathcal{Z}}{\text{minimize}} \left[\begin{array}{lll} \underset{(\rho^p,\,\rho^r)\geq 0}{\text{maximum}} & \displaystyle\sum_{i=1}^{K}\rho_i^p\left[f^T\lambda^{p,i}+q^T(u^{+,p,i}-u^{-,p,i})\right] & \\ & \quad\displaystyle+\sum_{j=1}^{L}\rho_j^r\left[f^T\lambda^{r,j}+q^T(u^{+,r,j}-u^{-,r,j})\right] & \\ \text{subject to} & \displaystyle\sum_{i=1}^{K}\rho_i^p\,\left[\,z^Tu^{+,p,i}+(\mathbf{1}-z)^Tv^{p,i}\,\right] & \\ & \quad\displaystyle+\sum_{j=1}^{L}\rho_j^r\,\left[\,z^Tu^{+,r,j}+(\mathbf{1}-z)^Tv^{r,j}\,\right]\,\leq\,0 & \\ \text{and} & \displaystyle\sum_{i=1}^{K}\rho_i^p\,=\,1, & \end{array}\right] \tag{3.14}$$

which is the *master IP*. It turns out that, after defining a new subset of extreme rays:

$$\mathcal{L}\,\equiv\,\left\{\,j\,\in\,\{\,1,\cdots,L\,\}\,:\,f^T\lambda^{r,j}+q^T(u^{+,r,j}-u^{-,r,j})\,>\,0\,\right\},$$

we can redefine the set $\mathcal{Z}$, which describes the feasible pieces of the LPCC, in terms of the extreme rays. The following proposition shows that the set $\mathcal{Z}$ can be described in terms of satisfiability inequalities that are constructed from the extreme rays in $\mathcal{L}$.

Proposition 5. $\mathcal{Z}=\left\{z\in\{0,1\}^m\,:\,\displaystyle\sum_{\ell:u_\ell^{+,r,j}>0}z_\ell+\sum_{\ell:v_\ell^{r,j}>0}(\,1-z_\ell\,)\,\geq\,1,\;\forall\,j\,\in\,\mathcal{L}\right\}.$

Proof. First of all, we can reformulate $\varphi_0(z)$ as

$$\begin{array}{ll} \underset{\rho^r\geq 0}{\text{maximize}} & \displaystyle\sum_{j=1}^{L}\rho_j^r\left[\,f^T\lambda^{r,j}+q^T(\,u^{+,r,j}-u^{-,r,j}\,)\right] \\ \text{subject to} & \displaystyle\sum_{j=1}^{L}\rho_j^r\,\left[\,z^Tu^{+,r,j}+(\mathbf{1}-z)^Tv^{r,j}\,\right]\,\leq\,0. \end{array}$$

For a given binary vector $z\,\in\,\{0,1\}^m$, the above maximization problem has a finite optimal solution if and only if z satisfies the constraints $\displaystyle\sum_{\ell:u_\ell^{+,r,j}>0}z_\ell+\sum_{\ell:v_\ell^{r,j}>0}(\,1-z_\ell\,)\,\geq\,1$ for all such extreme rays that $f^T\lambda^{r,j}+q^T(\,u^{+,r,j}-u^{-,r,j}\,)\,>\,0$. This is equivalent to saying that $z \in \mathcal{Z}$ if and only if such a z satisfies that

$$\sum_{\ell : u_\ell^{+,r,j} > 0} z_\ell + \sum_{\ell : v_\ell^{r,j} > 0} (1 - z_\ell) \geq 1 \quad \text{for all } \; j \in \mathcal{L}.$$

□

A corollary of Proposition 5 immediately follows and provides a certificate of infeasibility for the LPCC.

Corollary 6. If a subset $\mathcal{R}$ of $\mathcal{L}$ exists such that

$$\left\{ z \in \{0,1\}^m \, : \, \sum_{\ell : u_\ell^{+,r,j} > 0} z_\ell + \sum_{\ell : v_\ell^{r,j} > 0} (1 - z_\ell) \geq 1, \; \forall j \in \mathcal{R} \right\} = \emptyset,$$

then the LPCC (3.1) is infeasible.

Proof. Since $\mathcal{R} \subseteq \mathcal{L}$, we know that

$$\left\{ z \in \{0,1\}^m \, : \, \sum_{\ell : u_\ell^{+,r,j} > 0} z_\ell + \sum_{\ell : v_\ell^{r,j} > 0} (1 - z_\ell) \geq 1, \; \forall j \in \mathcal{L} \right\} = \emptyset.$$

It follows from Proposition 5 that $\mathcal{Z} = \emptyset$. Thus the infeasibility of the LPCC can be verified based on Theorem 4(a). □

Proposition 5 implies that (3.14) is equivalent to:

$$\underset{z \in \mathcal{Z}}{\text{minimize}} \left[\begin{array}{ll} \underset{\rho^p \geq 0}{\text{maximum}} & \displaystyle\sum_{i=1}^{K} \rho_i^p \left[f^T \lambda^{p,i} + q^T (u^{+,p,i} - u^{-,p,i}) \right] \\ \text{subject to} & \displaystyle\sum_{i=1}^{K} \rho_i^p \left[z^T u^{+,p,i} + (\mathbf{1} - z)^T v^{p,i} \right] \leq 0 \\ \text{and} & \displaystyle\sum_{i=1}^{K} \rho_i^p = 1 \end{array} \right]. \tag{3.15}$$

Note that the LPCC (3.1) is equivalent to this new problem (3.15). Especially, if the LPCC is known to attain finite optima, the $\text{LPCC}_{\min}$ is then given by the extreme point that yields the least objective value and satisfies the constraint $z^T u^{+,p} + (\mathbf{1} - z)^T v^p \leq 0$.

Similar to the inequality:

$$\sum_{\ell : u_\ell^{+,r,j} > 0} z_\ell + \sum_{\ell : v_\ell^{r,j} > 0} (1 - z_\ell) \geq 1,$$

which we call a *ray cut* (because it is induced by an extreme ray), we will construct a *point cut*:

$$\sum_{\ell : u_\ell^{+,p,i} > 0} z_\ell + \sum_{\ell : v_\ell^{p,i} > 0} (1 - z_\ell) \geq 1,$$

from an extreme point $(\lambda^{p,i}, u^{\pm,p,i}, v^{p,i})$ of Ξ chosen from the following collection:

$$\mathcal{K} \equiv \left\{ i \in \{1, \cdots, K\} : f^T\lambda^{p,i} + q^T(u^{+,p,i} - u^{-,p,i}) = \varphi(z) \text{ for some } z \in \mathcal{Z} \right\}.$$

Note that $\mathcal{K} \neq \emptyset \Rightarrow \mathcal{Z} \neq \emptyset$ (since $\mathcal{K}$ is a subset of $\mathcal{Z}$), which in turn implies that the LPCC (3.1) is feasible. Moreover, we have

$$\min_{i \in \mathcal{K}} \left[f^T\lambda^{p,i} + q^T(u^{+,p,i} - u^{-,p,i}) \right] \geq \text{LPCC}_{\min},$$

where the equality holds when the LPCC (3.1) is known to attain an optimal solution. For a given pair of subsets $\mathcal{P} \times \mathcal{R} \subseteq \mathcal{K} \times \mathcal{L}$, by letting

$$\mathcal{Z}(\mathcal{P}, \mathcal{R}) \equiv \left\{ \begin{array}{ll} z \in \{0,1\}^m : & \displaystyle\sum_{\ell : u_\ell^{+,r,j} > 0} z_\ell + \sum_{\ell : v_\ell^{r,j} > 0} (1 - z_\ell) \geq 1, \ \forall j \in \mathcal{R} \\ & \displaystyle\sum_{\ell : u_\ell^{+,p,i} > 0} z_\ell + \sum_{\ell : v_\ell^{p,i} > 0} (1 - z_\ell) \geq 1, \ \forall i \in \mathcal{P} \end{array} \right\},$$

we obtain the following proposition and a corollary in response to it.

Proposition 7. If there exists $\mathcal{P} \times \mathcal{R} \subseteq \mathcal{K} \times \mathcal{L}$ such that

$$\min_{i \in \mathcal{P}} \left[f^T\lambda^{p,i} + q^T(u^{+,p,i} - u^{-,p,i}) \right] > \text{LPCC}_{\min},$$

then $\operatorname*{argmin}_{z \in \mathcal{Z}} \varphi(z) \subseteq \mathcal{Z}(\mathcal{P}, \mathcal{R})$.

Proof. The proposition is obviously true when $\mathcal{Z}$ is an empty set. Let $\mathcal{Z} \neq \emptyset$ and $\widetilde{z} \in \mathcal{Z}$ be a minimizer of $\varphi(z)$ on $\mathcal{Z}$. Since $\widetilde{z}$ is an element of $\mathcal{Z}$, we can induce from Proposition 5 that $\widetilde{z} \in \mathcal{Z}(\emptyset, \mathcal{R})$. If $\widetilde{z} \notin \mathcal{Z}(\mathcal{P}, \mathcal{R})$, then there exists $i \in \mathcal{P}$ such that

$$\sum_{\ell: u_\ell^{+,p,i} > 0} \widetilde{z}_\ell + \sum_{\ell: v_\ell^{p,i} > 0} (1 - \widetilde{z}_\ell) = 0.$$

Hence, $(\lambda^{p,i}, u^{\pm,p,i}, v^{p,i})$ is feasible to the LP (3.9) corresponding to $\varphi(\widetilde{z})$; thus

$$\text{LPCC}_{\min} = \varphi(\widetilde{z}) \geq f^T \lambda^{p,i} + q^T (u^{+,p,i} - u^{-,p,i}) > \text{LPCC}_{\min},$$

which leads to a contradiction. □

Corollary 8. If there exists $\mathcal{P} \times \mathcal{R} \subseteq \mathcal{K} \times \mathcal{L}$ with $\mathcal{P} \neq \emptyset$ such that $\mathcal{Z}(\mathcal{P}, \mathcal{R}) = \emptyset$, then

$$\text{LPCC}_{\min} = \min_{i \in \mathcal{P}} \left[f^T \lambda^{p,i} + q^T (u^{+,p,i} - u^{-,p,i}) \right] \in (-\infty, \infty). \tag{3.16}$$

Proof. Suppose the equality does not hold in (3.16), then $\operatorname*{argmin}_{z \in \mathcal{Z}} \varphi(z) = \emptyset$, which implies $\mathcal{Z} = \emptyset$. This contradicts the assumption that $\mathcal{P} \neq \emptyset$. □

Combining Corollaries 6 and 8, we obtain the following restatement of Theorem 4 in terms of the extreme points and rays of Ξ.

Theorem 9. The following three statements hold:

(a) the LPCC (3.1) is infeasible if and only if a subset $\mathcal{R} \subseteq \mathcal{L}$ exists such that $\mathcal{Z}(\emptyset, \mathcal{R}) = \emptyset$;

(b) the LPCC (3.1) is feasible and has an unbounded objective if and only if $\mathcal{Z}(\mathcal{K}, \mathcal{L}) \neq \emptyset$;

(c) the LPCC (3.1) attains a finite optimal objective value if and only if a pair $\mathcal{P} \times \mathcal{R} \subseteq \mathcal{K} \times \mathcal{L}$ exists with $\mathcal{P} \neq \emptyset$ such that $\mathcal{Z}(\mathcal{P}, \mathcal{R}) = \emptyset$.

Proof. Statement (a) follows immediately from Corollary 6 by noting that $\mathcal{Z} = \mathcal{Z}(\emptyset, \mathcal{L}) \subseteq \mathcal{Z}(\emptyset, \mathcal{R})$. To prove the "if" part of (b), suppose $\mathcal{Z}(\mathcal{K}, \mathcal{L}) \neq \emptyset$. Let $\widehat{z} \in \mathcal{Z}(\mathcal{K}, \mathcal{L})$, then $\widehat{z} \in \mathcal{Z}$ and $\varphi_0(\widehat{z}) = 0$. Now we only need to prove that $\varphi(\widehat{z}) = -\infty$; i.e., the LP (3.9) corresponding to $\widehat{z}$ is infeasible. Assume otherwise, then $\varphi(\widehat{z})$ must attain a finite value, since $\varphi_0(\widehat{z}) = 0$. Hence there exists an extreme point $(\lambda^{p,i}, u^{\pm,p,i}, v^{p,i})$ of the LP (3.9) corresponding to $\widehat{z}$ such that $f^T \lambda^{p,i} + q^T (u^{+,p,i} - u^{-,p,i}) = \varphi(\widehat{z})$, and satisfies that

$\widehat{z}^T u^{+,p,i} + (\mathbf{1} - \widehat{z})^T v^{p,i} \leq 0$. This is not possible since $i \in \mathcal{K}$, which implies that $\widehat{z}$ must satisfy

$$\sum_{\ell : u_\ell^{+,p,i} > 0} \widehat{z}_\ell + \sum_{\ell : v_\ell^{p,i} > 0} (1 - \widehat{z}_\ell) \geq 1.$$

Therefore, the LPCC (3.1) is feasible and unbounded below on any piece that is defined by $z \in \mathcal{Z}(\mathcal{K}, \mathcal{L})$. Conversely, suppose $\text{LPCC}_{\min} = -\infty$. By Theorem 4, there exists a binary vector $\widehat{z} \in \mathcal{Z}$ such that $\varphi(\widehat{z}) = -\infty$; i.e., the LP (3.9) corresponding to $\widehat{z}$ is infeasible. In turn, this means that $\widehat{z}^T u^{+,p,i} + (\mathbf{1} - \widehat{z})^T v^{p,i} > 0$, for all $i = 1, \cdots, K$; or equivalently,

$$\sum_{\ell : u_\ell^{+,p,i} > 0} \widehat{z}_\ell + \sum_{\ell : v_\ell^{p,i} > 0} (1 - \widehat{z}_\ell) \geq 1,$$

for all $i = 1, \cdots, K$. Since we already know that $\widehat{z} \in \mathcal{Z} = \mathcal{Z}(\emptyset, \mathcal{L})$, it follows that $\widehat{z} \in \mathcal{Z}(\mathcal{K}, \mathcal{L})$. Hence, statement (b) holds. Finally, the "if" statement in (c) follows from Corollary 8. Conversely, if the LPCC (3.1) has a finite optimal solution, then by (b), it follows that $\mathcal{Z}(\mathcal{K}, \mathcal{L}) = \emptyset$. Since the LPCC (3.1) is feasible, $\mathcal{K} \neq \emptyset$ by (a), establishing the "only if" part of (c). $\square$

Theorem 9 provides the theoretical basis for the algorithm to be presented in Section 3.4 for resolving the LPCCs. Through the successive generation of extreme points and rays of Ξ, the algorithm can be terminated with a pair of subsets $\mathcal{P} \times \mathcal{R}$ of $\mathcal{K} \times \mathcal{L}$ such that $\mathcal{Z}(\mathcal{P}, \mathcal{R}) = \emptyset$. With such a pair successfully identified, the original LPCC (3.1) is either infeasible ($\mathcal{P} = \emptyset$) or feasible with a finite optimal solution ($\mathcal{P} \neq \emptyset$). If no such pair exists, then the LPCC (3.1) is unbounded. Especially, the piece on which the LPCC is unbounded below can be identified by finding a binary vector $z \in \mathcal{Z}$ such that $\varphi(z) = -\infty$, i.e., the LP (3.9) is infeasible. Based on the point/ray cuts constructed from the finite number of extreme point/ray of the set Ξ, the algorithm can be shown to terminate in finite time.

3.3 Simple Cuts and Sparsification

In this section, we will explain several key steps implemented in our algorithm in order to improve the efficiency. The first key step, named by *simple cut*, is a version of the well-known Gomory cut in integer programming specialized to the LPCC. This step was first employed for solving bilevel LPs; see [5]. The second idea aims at "sparsifying" the ray/point cuts to facilitate the computation of the IPs which are defined by the constraints from the working sets $\mathcal{Z}(\mathcal{P},\mathcal{R})$. Specifically, we say that a satisfiability constraint:

$$\sum_{i \in \mathcal{I}'} z_i + \sum_{j \in \mathcal{J}'} (1 - z_j) \geq 1 \quad \text{is } \textit{sparser} \text{ than} \quad \sum_{i \in \mathcal{I}} z_i + \sum_{j \in \mathcal{J}} (1 - z_j) \geq 1,$$

if $\mathcal{I}' \subseteq \mathcal{I}$ and $\mathcal{J}' \subseteq \mathcal{J}$. In general, a satisfiability inequality cuts off certain LP pieces of the LPCC; i.e., the constraint $z_1 \geq 1$ cuts off the LP pieces with $z_1 = 0$. The sparser the inequality is, the more pieces it cuts off. Thus, it is desirable to sparsify a cut as much as possible. However, sparsification requires more computational work on the solution of linear subprograms; thus one needs to balance the work required with the benefit of the process.

3.3.1 Simple cuts

The following discussion presents the *simple cut* and how it is used to obtain tighter relaxed linear programs obtained by dropping the complementarity conditions in the LPCC (3.1). This method was first investigated in [5] in order to facilitate the branch-and-cut algorithm for resolving bilevel LPs. Consider the LP relaxation of the LPCC (3.1):

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & c^T x + d^T y \\ \text{subject to} & Ax + By \geq f \\ \text{and} & 0 \leq y, \quad w \equiv q + Nx + My \geq 0, \end{array} \tag{3.17}$$

where the orthogonal condition $y^T w = 0$ has been dropped. Assume that the LP (3.17) is bounded below and the optimal solution fails the orthogonality condition, say $y_i w_i > 0$. Then, y_i and w_i must be the basic variables in the obtained solution; suppose the expressions of w_i and y_i in the optimal tableau are, respectively:

$$w_i = w_{i0} - \sum_{s_j:\text{nonbasic}} a_j s_j \quad \text{and} \quad y_i = y_{i0} - \sum_{s_j:\text{nonbasic}} b_j s_j$$

with $\min(w_{i0}, y_{i0}) > 0$. To follow the reference [5], we assume that the variables in (3.17) are restricted in nonnegative orthant (Note that x can be written as the difference of two nonnegative slack variables). It has been shown in [5] that the following inequality must be satisfied by all feasible solutions of the LPCC (3.1)

$$\sum_{\substack{s_j \,:\ \text{nonbasic} \\ \max(a_j, b_j) > 0}} \max\left(\frac{a_j}{w_{i0}}, \frac{b_j}{y_{i0}}\right) s_j \geq 1. \tag{3.18}$$

If $a_j \leq 0$ for all nonbasic j, then $w_i > 0 = y_i$ for every feasible solution of the LPCC (3.1). A similar remark can be made if $b_j \leq 0$ for all nonbasic j.

Following the terminology used in [5], we call the inequality (3.18) a *simple cut*. Multiple such cuts can be generated based on the solution of the LP (3.17); we can add even more simple cuts into the constraint set $Ax + By \geq f$ by repeating this procedure. As a result, we obtain a modified inequality $\widetilde{A}x + \widetilde{B}y \geq \widetilde{f}$ in the LPCC (3.1). This strategy turns out to be a very effective pre-processor for the overall algorithm for resolving LPCCs. At the end of this pre-processor, the obtained optimal solution $(\bar{x}, \bar{y}, \bar{w})$ of (3.17) still fails the orthogonal condition of the LPCC (otherwise, this solution would be optimal to the LPCC already); the optimal objective value $c^T\bar{x} + d^T\bar{y}$ provides a valid lower bound for $\text{LPCC}_{\min}$. (Note: if (3.17) is unbounded, then the pre-processor does not produce any cuts or a finite lower bound.)

LPCC feasibility recovery

We will have a further discussion about a special case $B = 0$, which occurs in many applications. Suppose that the solution $(\bar{x}, \bar{y}, \bar{w})$ is obtained from the simple-cut pre-processor. The vector $\bar{x}$ can be used to produce a feasible solution to the LPCC (3.1) by simply solving the linear complementarity problem (LCP): $0 \leq y \perp q + N\bar{x} + My \geq 0$ (assuming that the matrix M has favorable properties such that this step is effective). Let $\bar{y}'$ be a solution to the LCP. The pair $(\bar{x}, \bar{y}')$ is feasible to the LPCC (3.1), thus the objective value $c^T\bar{x} + d^T\bar{y}'$ yields a valid upper bound to $\text{LPCC}_{\min}$. Note that the modified matrix $\widetilde{B}$ obtained from the pre-processer is not necessarily zero. Nevertheless, we can still apply this recovery procedure since any feasible solution of the LCP will satisfy the modified constraints. This recovery procedure can be extended to the case where

$B \neq 0$. Incidentally, this class of LPCCs is generally "more difficult" than the class where $B = 0$, where the difficulty is determined by our empirical experience from the computational tests. Let $(\bar{x}, \bar{y}, \bar{w})$ be the optimal solution to the LP (3.17), that fails the orthogonal condition. A feasible solution to the LPCC could be recovered by either solving the LP(α), where $\alpha \equiv \{i : \bar{y}_i \leq \bar{w}_i\}$, or by solving $\varphi(z)$, where $z_\alpha = 1$ and $z_{\bar{\alpha}} = 0$. The optimal solution of LP(α), if it exists (possibly this LP is infeasible; in this case, the recovery step is ineffective), yields a finite upper bound for LPCC$_{\min}$. In general, there is no guarantee that this procedure will always be successful; nevertheless, it is very effective when it works.

3.3.2 Cut management

Another key step in our algorithm is regarding the selection of the constraints contained in the working set $\mathcal{Z}(\mathcal{P}, \mathcal{R})$. Since the constraints in $\mathcal{Z}(\mathcal{P}, \mathcal{R})$ are of the satisfiability type, some special algorithms could be employed (see [8, 40] and the references therein for some such algorithms). We have developed a special heuristic that utilizes a valid upper bound of LPCC$_{\min}$ to sparsify the terms in the ray/point cuts in the working set $\mathcal{Z}(\mathcal{P}, \mathcal{R})$. In what follows, we describe how the algorithm manages these cuts.

To begin, we define three pools of cuts, labeled $\mathcal{Z}_{\text{work}}$–the working pool, $\mathcal{Z}_{\text{wait}}$–the wait pool, and $\mathcal{Z}_{\text{cand}}$–the candidate pool. The decision of whether or not to sparsify a valid inequality is made according to a current LPCC upper bound and a small scalar $\delta > 0$. The sub-inequalities, which are obtained from the sparsification of those cuts in $\mathcal{Z}(\mathcal{P}, \mathcal{R})$, are placed in $\mathcal{Z}_{\text{cand}}$ to be validated later; this set always turns to be empty at the end of the sparsification procedure. $\mathcal{Z}_{\text{work}}$ contains the valid sub-inequalities, while $\mathcal{Z}_{\text{wait}}$ contains the constraints that are not valid yet and may be validated later. We denote the set of the binary vectors that satisfy the constraints in $\mathcal{Z}_{\text{work}}$ as $\widehat{\mathcal{Z}}_{\text{work}}$. In essence, the sparsification is an effective way to facilitate the search for a binary vector feasible to $\widehat{\mathcal{Z}}_{\text{work}}$, since it is computationally more difficult to find feasible solutions satisfying many dense inequalities. Especially, a sparsest inequality with only one term in it automatically fixes one complementarity; e.g., $z_1 \geq 1$ fixes $w_1 = 0$.

Suppose the inequality to be sparsified is given by

$$\sum_{i \in \mathcal{I}} z_i + \sum_{j \in \mathcal{J}} (1 - z_j) \geq 1. \tag{3.19}$$

Partition the set $\mathcal{I}$ into two disjoint subsets $\mathcal{I}_1$ and $\mathcal{I}_2$, i.e., $\mathcal{I} = \mathcal{I}_1 \cup \mathcal{I}_2$ and $\mathcal{I}_1 \cap \mathcal{I}_2 = \emptyset$; similarly, let $\mathcal{J} = \mathcal{J}_1 \cup \mathcal{J}_2$ and $\mathcal{J}_1 \cap \mathcal{J}_2 = \emptyset$. We split (3.19), which we call the *parent*, into two sub-inequalities:

$$\sum_{i \in \mathcal{I}_1} z_i + \sum_{j \in \mathcal{J}_1} (1 - z_j) \geq 1 \quad \text{and} \quad \sum_{i \in \mathcal{I}_1} z_i + \sum_{j \in \mathcal{J}_2} (1 - z_j) \geq 1; \tag{3.20}$$

and test both to see if they are valid cuts for $\mathcal{Z}_{\text{work}}$. Denote the current upper bound for the LPCC as LPCC_{ub}. To test the left-hand inequality, we consider the LP relaxation (3.17) with fixed variables $w_i = (q + Nx + My)_i = 0$ for $i \in \mathcal{I}_1$ and $y_i = 0$ for $i \in \mathcal{J}_1$. Such an LP is named by a *relaxed LP with restriction*. If the optimal objective value of this LP is no less than LPCC_{ub}, then we have successfully sparsified the inequality (3.19) into the sparser inequality:

$$\sum_{i \in \mathcal{I}_1} z_i + \sum_{j \in \mathcal{J}_1} (1 - z_j) \geq 1, \tag{3.21}$$

which proves to be a valid cut for $\mathcal{Z}_{\text{work}}$. Otherwise, we can apply the LPCC feasibility recovery procedure and recovery a feasible solution to the LPCC, which may or may not improve LPCC_{ub}. More specifically, there are two cases happening: if the objective value of this recovered solution is no less than LPCC_{ub}, then we can generate a new cut for $\mathcal{Z}_{\text{work}}$; otherwise, we have successfully reduced the LPCC upper bound. Either case, we obtain positive progress in the algorithm. Moreover, we save the cut (3.21) in the wait pool $\mathcal{Z}_{\text{wait}}$ for later consideration. A similar procedure can be applied to the right-hand inequality. Cuts in the wait pool are not yet proven to be valid for the LPCC. In order to revisit them when there is a reduction of LPCC_{ub} in the process, we associate each inequality in $\mathcal{Z}_{\text{wait}}$ with an objective value, which should be strictly less than the current LPCC upper bound.

In our experiment, the sets $\mathcal{I}$ and $\mathcal{J}$ are randomly divided into two roughly equal halves respectively. The following illustrates one such division:

$$\begin{array}{ccc} & z_1 + z_3 + z_4 + (1 - z_2) + (1 - z_6) \geq 1 & \\ \swarrow & & \searrow \\ z_1 + z_3 + (1 - z_2) \geq 1 & & z_4 + (1 - z_6) \geq 1. \end{array}$$

To maximize the effect of the sparsification procedure, we adopt a procedure that attempts to sparsify the *root inequality* (3.19) as much as possible. We use a small scalar $\delta > 0$ to help decide whether or not to conduct further branching. In essence, we only branch if the inequality appears to have a better chance to be successfully sparsified. The sparsification procedure is described in detail as follows.

Sparsification procedure. Let (3.19) be the root inequality to be sparsified, LPCC_{ub} be the current LPCC upper bound, and $\delta > 0$ be a given scalar. Branch (3.19) into two sub-inequalities (3.20), both of which we put in the set $\mathcal{Z}_{\text{cand}}$.

Main step. If $\mathcal{Z}_{\text{cand}}$ is empty, terminate. Otherwise pick a *candidate* inequality in $\mathcal{Z}_{\text{cand}}$, say the left one in (3.20) with the corresponding pair of index sets $(\mathcal{I}_1, \mathcal{J}_1)$. Solve the LP relaxation (3.17) of the LPCC (3.1) with the additional constraints $w_i = (q + Nx + My)_i = 0$ for $i \in \mathcal{I}_1$ and $y_i = 0$ for $i \in \mathcal{J}_1$, obtaining an LP optimal objective value, say $\text{LP}_{\text{rlx}} \in \Re \cup \{\pm\infty\}$. We have the following three cases.

• If $\text{LP}_{\text{rlx}} \in [\,\text{LPCC}_{\text{ub}}, \text{LPCC}_{\text{ub}} + \delta\,]$, move the candidate inequality from $\mathcal{Z}_{\text{cand}}$ into $\mathcal{Z}_{\text{work}}$ and remove its parent from $\mathcal{Z}_{\text{work}}$; return to the main step.

• If $\text{LP}_{\text{rlx}} < \text{LPCC}_{\text{ub}}$, apply the LPCC feasibility recovery procedure to the optimal solution of the current relaxed LP with restriction; and obtain either a new cut or a reduced LPCC_{ub}. Move the incumbent candidate inequality from $\mathcal{Z}_{\text{cand}}$ into $\mathcal{Z}_{\text{wait}}$; return to the main step.

• If $\delta + \text{LPCC}_{\text{ub}} < \text{LP}_{\text{rlx}}$, move the candidate inequality from $\mathcal{Z}_{\text{cand}}$ into $\mathcal{Z}_{\text{work}}$ and remove its parent; further branch the candidate inequality into two sub-inequalities, both of which we put into the candidate pool $\mathcal{Z}_{\text{cand}}$; return to the main step.

During the procedure, the set $\mathcal{Z}_{\text{cand}}$ may grow with subsequent branching; and eventually shrinks to empty. If the sparsification is successful, we have obtained several valid sparser cuts, which will facilitate the computation of a feasible solution to $\mathcal{Z}_{\text{work}}$. Otherwise some sparser cuts are added into $\mathcal{Z}_{\text{wait}}$, waiting to be validated in subsequent iterations. Note that associated with each inequality in $\mathcal{Z}_{\text{wait}}$ is the value LP_{rlx}.

3.4 The IP Algorithm

Now we are ready to present the parameter-free IP-based algorithm for resolving an arbitrary LPCC (3.1). Afterwards we will show that the algorithm can be successfully terminated within a finite number of *iterations* with a definitive resolution of the LPCC in one of its three states. Referring to a return to Step 1, each iteration consists of solving one feasibility IP of the satisfiability kind, a couple LPs to compute $\varphi(\widehat{z})$ and possibly $\varphi_0(\widehat{z})$ corresponding to a binary vector $\widehat{z}$ obtained from the IP, and multiple LPs within the sparsification procedure associated with a point(ray) cut derived from the solution of $\varphi(\widehat{z})$ ($\varphi_0(\widehat{z})$).

The algorithm

- *Step 0.* (Preprocessing and initialization) Generate multiple simple cuts to tighten the feasible set of the relaxed LP. If any of the LPs encountered in this step is infeasible, so is the LPCC (3.1). In general, let LPCC_{lb} (set to be $-\infty$) and LPCC_{ub} (set to be ∞) be valid lower and upper bounds of $\text{LPCC}_{\min}$, respectively. Let $\delta > 0$ be a small scalar. [A finite optimal solution to a relaxed LP provides a finite lower bound, and a feasible solution to the LPCC, which could be obtained from the LPCC feasibility recovery procedure, provides a finite upper bound.] Set $\mathcal{P} = \mathcal{R} = \emptyset$ and $\mathcal{Z}_{\text{work}} = \mathcal{Z}_{\text{wait}} = \emptyset$. Thus, $\widehat{\mathcal{Z}}_{\text{work}} = \{0,1\}^m$.

- *Step 1.* (Solving a satisfiability IP) Determine a vector $\widehat{z} \in \widehat{\mathcal{Z}}_{\text{work}}$. If this set is empty, go to Step 2. Otherwise go to Step 3.

- *Step 2.* (Termination: infeasibility or finite solvability) If $\mathcal{P} = \emptyset$, we have obtained a certificate of infeasibility for the LPCC (3.1); stop. If $\mathcal{P} \neq \emptyset$, we have obtained a certificate of global optimality for the LPCC (3.1) with $\text{LPCC}_{\min}$ given by (3.16); stop.

- *Step 3.* (Solving dual LP) Compute $\varphi(\widehat{z})$ by solving the LP (3.9). If $\varphi(\widehat{z}) \in$

$(-\infty, \infty)$, go to Step 4a. If $\varphi(\widehat{z}) = \infty$, proceed to Step 4b. If $\varphi(\widehat{z}) = -\infty$, proceed to Step 4c.

- *Step 4a.* (Adding an extreme point) Let $(\lambda^{p,i}, u^{\pm,p,i}, v^{p,i}) \in \mathcal{K}$ be an optimal extreme point of Ξ. There are 3 cases.

  (1) If $\varphi(\widehat{z}) \in [\,\text{LPCC}_{\text{ub}},\ \text{LPCC}_{\text{ub}} + \delta]$, let $\mathcal{P} \leftarrow \mathcal{P} \cup \{i\}$ and add the corresponding point cut to $\mathcal{Z}_{\text{work}}$; return to Step 1.

  (2) If $\varphi(\widehat{z}) > \text{LPCC}_{\text{ub}} + \delta$, let $\mathcal{P} \leftarrow \mathcal{P} \cup \{i\}$ and add the corresponding point cut to $\mathcal{Z}_{\text{work}}$. Apply the sparsification procedure to the new point cut, obtaining an updated $\mathcal{Z}_{\text{work}}$ and $\mathcal{Z}_{\text{wait}}$, and possibly a reduced LPCC_{ub}. If the LPCC upper bound is reduced during the sparsification procedure, go to Step 5 to activate some of the cuts in the wait pool; otherwise, return to Step 1.

  (3) If $\varphi(\widehat{z}) < \text{LPCC}_{\text{ub}}$, let $\text{LPCC}_{\text{ub}} \leftarrow \varphi(\widehat{z})$ and go to Step 5.

- *Step 4b.* (Adding an extreme ray) Let $(\lambda^{r,j}, u^{\pm,r,j}, v^{r,j}) \in \mathcal{L}$ be an extreme ray of Ξ. Set $\mathcal{R} \longleftarrow \mathcal{R} \cup \{j\}$ and add the corresponding ray cut to $\mathcal{Z}_{\text{work}}$. Apply the sparsification procedure to the new ray cut, obtaining an updated $\mathcal{Z}_{\text{work}}$ and $\mathcal{Z}_{\text{wait}}$, and possibly a reduced LPCC_{ub}. If the LPCC upper bound is reduced during the sparsification procedure, go to Step 5 to activate some of the cuts in the wait pool; otherwise, return to Step 1.

- *Step 4c.* (Determining LPCC unboundedness) Solve the LP (3.10) to determine $\varphi_0(z)$. If $\varphi_0(z) = 0$, then the vector z and its support provide a certificate of unboundedness for the LPCC (3.1). Stop. If $\varphi_0(z) = \infty$, go to Step 4b.

- *Step 5.* Move all inequalities in $\mathcal{Z}_{\text{wait}}$ with values LP_{rlx} greater than (the just reduced) LPCC_{ub} into $\mathcal{Z}_{\text{work}}$. Apply the sparsification procedure to each newly moved inequality with $\text{LP}_{\text{rlx}} >\ \text{LPCC}_{\text{ub}} + \delta$. Re-apply this step to the cuts in $\mathcal{Z}_{\text{wait}}$ each time the LPCC upper bound is reduced from the sparsification procedure. Return to Step 1 when no more cuts in $\mathcal{Z}_{\text{wait}}$ are eligible for sparsification.

Theorem 10. The algorithm terminates in a finite number of iterations.

Proof. The finiteness is due to the following observations: (a) the set of m-dimensional binary vectors is finite, (b) each iteration of the algorithm generates a completely new binary vector that is distinct from all those previously generated, and (c) there are only finitely many cuts. (a) and (c) are obvious; (b) follows from the operation of the algorithm: at each iteration, a new obtained point cut or ray cut, combined with other inequalities in $\mathcal{Z}_{\text{work}}$, will cut off all binary vectors generated so far, including the current binary vector $\widehat{z}$. □

3.4.1 A numerical example

We use the following simple example to illustrate the algorithm:

$$\begin{array}{ll} \underset{(x,y)}{\text{minimize}} & x_1 + 2\,y_1 - y_3 \\ \text{subject to} & x_1 + x_2 \geq 5 \\ & x_1,\, x_2 \geq 0 \\ & 0 \leq y_1 \;\perp\; x_1 - y_3 + 1 \geq 0 \\ & 0 \leq y_2 \;\perp\; x_2 + y_1 + y_2 \geq 0 \\ & 0 \leq y_3 \;\perp\; x_1 + x_2 - y_2 + 2 \geq 0. \end{array} \tag{3.22}$$

Note that the LCP in the variable y is not derived from a convex quadratic program, since the matrix

$$M \equiv \begin{bmatrix} 0 & 0 & -1 \\ 1 & 1 & 0 \\ 0 & -1 & 0 \end{bmatrix}$$

is not positive semidefinite; although the matrix M has all principal minors nonnegative, the LCPs defined by this matrix may have zero or unbounded solutions.

Initialization: Set the upper bound as infinity, i.e., $\text{LPCC}_{\text{ub}} = \infty$. Set the working set $\mathcal{Z}_{\text{work}}$ and the waiting set $\mathcal{Z}_{\text{wait}}$ both to be empty.

Iteration 1: Since $\mathcal{Z}_{\text{work}}$ is an empty set, any binary vector would be feasible for $\widehat{\mathcal{Z}}_{\text{work}}$.

We choose $z = (0,0,0)$ and solve the dual LP (3.9):

$$
\begin{array}{lrcl}
\underset{(\lambda,u^{\pm},v)}{\text{maximize}} & 5\,\lambda + u_1^+ + 2\,u_3^+ - u_1^- - 2\,u_3^- & & \\
\text{subject to} & \lambda - u_1^+ + u_1^- - u_3^+ + u_3^- & \leq & 1 \\
& \lambda - u_2^+ + u_2^- - u_3^+ + u_3^- & \leq & 0 \\
& -u_2^+ + u_2^- - v_1 & \leq & 2 \\
& -u_2^+ + u_2^- + u_3^+ - u_3^- - v_2 & \leq & 0 \\
& u_1^+ - u_1^- - v_3 & \leq & -1 \\
& v_1 + v_2 + v_3 & \leq & 0 \\
& (\,\lambda, u^{\pm}, v\,) \geq 0, & &
\end{array}
\tag{3.23}
$$

which is unbounded, yielding an extreme ray with $u^+ = (0, 10/7, 10/7)$ and $v = (0,0,0)$ and a corresponding ray cut: $z_2 + z_3 \geq 1$. (Briefly, this cut is valid since $z_2 = z_3 = 0$ implies both $x_2 + y_1 + y_2 = 0$ and $x_1 + x_2 - y_2 + 2 = 0$, which can't both hold for nonnegative x and y.) Add this cut to $\mathcal{Z}_{\text{work}}$ and initiate the sparsification procedure. This inequality $z_2 + z_3 \geq 1$ can be branched into: $z_2 \geq 1$ or $z_3 \geq 1$. To test if $z_2 \geq 1$ is a valid cut, we form the following relaxed LP of (3.22) by restricting $x_2 + y_1 + y_2 = 0$:

$$
\begin{array}{lll}
\underset{(x,y)}{\text{minimize}} & x_1 + 2\,y_1 - y_3 & \\
\text{subject to} & x_1 + x_2 & \geq\ 5 \\
& x_1 - y_3 + 1 & \geq\ 0 \\
& x_2 + y_1 + y_2 & =\ 0 \\
& x_1 + x_2 - y_2 + 2 & \geq\ 0 \\
& x,\, y \geq 0. &
\end{array}
\tag{3.24}
$$

An optimal solution of the LP (3.24) is $(x_1, x_2, y_1, y_2, y_3) = (5,0,0,0,6)$ with the optimal objective value $\text{LP}_{\text{rlx}} = -1$. This is not a feasible solution of the LPCC (3.22) because the third complementarity is violated. The inequality $z_2 \geq 1$ is therefore placed in the waiting set $\mathcal{Z}_{\text{wait}}$. We then use $(x_1, x_2) = (5, 0)$ to recover an LPCC feasible solution by solving the LCP in the variable y. This yields $y = (0,0,0)$ and $w = (6,0,7)$, and hence a corresponding vector $z = (1,0,1)$. Using this z in (3.9), we get another dual problem:

$$\begin{array}{lrcr}
\underset{(\lambda,u^{\pm},v)}{\text{maximize}} & 5\,\lambda + u_1^+ + 2\,u_3^+ - u_1^- - 2\,u_3^- & & \\
\text{subject to} & \lambda - u_1^+ + u_1^- - u_3^+ + u_3^- & \leq & 1 \\
& \lambda - u_2^+ + u_2^- - u_3^+ + u_3^- & \leq & 0 \\
& -u_2^+ + u_2^- - v_1 & \leq & 2 \\
& -u_2^+ + u_2^- + u_3^+ - u_3^- - v_2 & \leq & 0 \\
& u_1^+ - u_1^- - v_3 & \leq & -1 \\
& u_1^+ + v_2 + u_3^+ & \leq & 0 \\
& (\,\lambda, u^{\pm}, v\,) \geq 0, & &
\end{array} \tag{3.25}$$

which has an optimal value 5 that is smaller than the current upper bound $\mathrm{LPCC_{ub}}$. So we update the upper bound as $\mathrm{LPCC_{ub}} = 5$. Note that this update occurs during the sparsification step. A corresponding optimal solution to (3.25) is $u^+ = (0,1,0)$ and $v = (0,0,1)$. Hence we can add the point cut: $z_2 + (1 - z_3) \geq 1$ to $\mathcal{Z}_{\mathrm{work}}$.

When we next proceed to the other branch: $z_3 \geq 1$, we have a relaxed LP:

$$\begin{array}{llcr}
\underset{(x,y)}{\text{minimize}} & x_1 + 2\,y_1 - y_3 & & \\
\text{subject to} & x_1 + x_2 & \geq & 5 \\
& x_1 - y_3 + 1 & \geq & 0 \\
& x_2 + y_1 + y_2 & \geq & 0 \\
& x_1 + x_2 - y_2 + 2 & = & 0 \\
& x,\, y \geq 0 & &
\end{array} \tag{3.26}$$

Solving (3.26) gives an optimal value $\mathrm{LP_{rlx}} = -1$, which is smaller than $\mathrm{LPCC_{ub}}$, and a violated complementarity with $w_2 = 12$ and $y_2 = 7$. Adding $z_3 \geq 1$ to $\mathcal{Z}_{\mathrm{wait}}$, we apply the LPCC feasibility recovering procedure to $x = (0,5)$, and get a new LPCC feasible piece with $z = (1,1,1)$. Substituting z into (3.9), we get another LP:

$$\begin{array}{lrcl}
\underset{(\lambda,u^{\pm},v)}{\text{maximize}} & 5\,\lambda + u_1^+ + 2\,u_3^+ - u_1^- - 2\,u_3^- & & \\
\text{subject to} & \lambda - u_1^+ + u_1^- - u_3^+ + u_3^- & \leq & 1 \\
 & \lambda - u_2^+ + u_2^- - u_3^+ + u_3^- & \leq & 0 \\
 & -u_2^+ + u_2^- - v_1 & \leq & 2 \\
 & -u_2^+ + u_2^- + u_3^+ - u_3^- - v_2 & \leq & 0 \\
 & u_1^+ - u_1^- - v_3 & \leq & -1 \\
 & u_1^+ + u_2^+ + u_3^+ & \leq & 0 \\
 & (\,\lambda, u^{\pm}, v\,) \geq 0 & &
\end{array} \tag{3.27}$$

which has an optimal objective value 0. So a better upper bound is found; thus $\text{LPCC}_{\text{ub}} = 0$. A point cut: $1-z_3 \geq 1$ is derived from an optimal solution of (3.27). This cut obviously implies the previous cut: $z_2 + (1 - z_3) \geq 1$. In order to reduce the work load of the IP solver, we can delete $z_2 + (1 - z_3) \geq 1$ from $\mathcal{Z}_{\text{work}}$ and add in $1 - z_3 \geq 1$ instead. So far, we have the updated upper bound: $\text{LPCC}_{\text{ub}} = 0$ and the working set $\mathcal{Z}_{\text{work}}$ defined by the two inequalities:

$$z_2 + z_3 \,\geq\, 1 \quad \text{and} \quad 1 - z_3 \,\geq\, 1. \tag{3.28}$$

This completes iteration 1. During this one iteration, we have solved 5 LPs, the LPCC_{ub} has improved twice, and we have obtained 2 valid cuts.

Iteration 2: Solving a satisfiability IP yields a $z = (0,1,0) \in \widehat{\mathcal{Z}}_{\text{work}}$. Indeed, any element in $\widehat{\mathcal{Z}}_{\text{work}}$, which is defined by the two inequalities in (3.28), must have $z_2 = 1$ and $z_3 = 0$; thus it remains to determine z_1. As it turns out, z_1 is irrelevant. To see this, we substitute

$z = (0, 1, 0)$ into (3.9), obtaining

$$\begin{array}{lrcr}
\underset{(\lambda, u^\pm, v)}{\text{maximize}} & 5\,\lambda + u_1^+ + 2\,u_3^+ - u_1^- - 2\,u_3^- & & \\
\text{subject to} & \lambda - u_1^+ + u_1^- - u_3^+ + u_3^- & \leq & 1 \\
& \lambda - u_2^+ + u_2^- - u_3^+ + u_3^- & \leq & 0 \\
& -u_2^+ + u_2^- - v_1 & \leq & 2 \\
& -u_2^+ + u_2^- + u_3^+ - u_3^- - v_2 & \leq & 0 \\
& u_1^+ - u_1^- - v_3 & \leq & -1 \\
& u_2^+ + v_1 + v_3 & \leq & 0 \\
& (\,\lambda, u^\pm, v\,) \geq 0. & &
\end{array} \tag{3.29}$$

The LP (3.29) is unbounded and has an extreme ray where $u^+ = (0, 0, 10/7)$ and $v = (0, 10/7, 0)$. So we can add a valid ray cut: $(1 - z_2) + z_3 \geq 1$ to $\mathcal{Z}_{\text{work}}$.

Termination: The updated working set $\mathcal{Z}_{\text{work}}$ consists of 3 inequalities:

$$\left\{ \begin{array}{rcl}
z_2 + z_3 & \geq & 1 \\
1 - z_3 & \geq & 1 \\
(1 - z_2) + z_3 & \geq & 1
\end{array} \right\},$$

which can be seen to be inconsistent. Hence we get a certificate of termination. Since there is one point cut in $\mathcal{Z}_{\text{work}}$, the LPCC (3.22) has an optimal objective value 0, which happens on the piece $z = (1, 1, 1)$. (This termination can be expected from the fact that $z_2 = 1$ and $z_3 = 0$ for elements in the set $\widehat{\mathcal{Z}}_{\text{work}}$ prior to the last ray cut; these values of z imply that $y_2 = w_3 = 0$, which are not consistent with the nonnegativity of x. This inconsistency is detected by the algorithm through the generation of a ray cut that leaves $\widehat{\mathcal{Z}}_{\text{work}}$ empty.) $\square$

3.5 Computational Results

We have coded our algorithm in MATLAB and used CPLEX 9.1 to solve the LPs and the satisfiability IPs. The experiments were run on a DELL desktop computer with 1.40GHz Pentium 4 processor and 1.00GB of RAM. The computational results are presented in the figures and tables attached at the end of this section. To test the effectiveness of our algorithm, we have implemented and compared it with benchmark algorithms FILTER and KNITRO which are publicly available from NEOS. As shown in the experiments, these two solvers have consistently produced LPCC feasible solutions with high-quality, most of which turned out to be globally optimal with the optimality verified by our algorithm. (The details can be seen in Tables 3.1, 3.2, and 3.3).

In this computational study, we have set the following three goals: (A) to test the ability of the algorithm to compute optimal solutions for solvable LPCCs and verify the global optimality of the computed solutions; (B) to determine the quality of the solutions obtained using the simple-cut pre-processor; and (C) to demonstrate that the algorithm is capable of detecting infeasibility and unboundedness for LPCCs of these two kinds. All problems are randomly generated. To test (A) and (B), the problems are generated to be feasible and have the objective value bounded below on its feasible region; for (C), the problems are generated to be either infeasible or feasible with unbounded objective values. The algorithm, however, does not make use of such information in any way; instead, it is up to the algorithm to verify the prescribed problem status. For each problem's preprocessing step, a total of $\lfloor m/3 \rfloor$ simple cuts are generated; a valid lower bound for each problem is obtained by solving the relaxed LP with these simple cuts. The optimality of the LPCC is declared if the difference between the lower and upper bound is less than or equal to 1e-6. This tolerance is also employed to determine if the relaxed LP solutions are feasible to the original LPCC. The parameter δ for the sparsification step is selected to be 0.2.

All problems have the nonnegativity constraint $x \geq 0$. The computational results for the problems with finite optima are reported in Figures 3.1, 3.2, and 3.3 and Tables 3.1, 3.2, and 3.3. Each figure contains one set of ten randomly generated problems with the same characteristics. Figures 3.1, 3.2, and 3.3 correspond to problems with $[n, m, k] = [100, 100, 90]$, $[300, 300, 200]$ and $[50, 50, 55]$, respectively. These sizes and the data density are dictated by the limitations of MATLAB that is the environment where our experiments were performed. All data are randomly generated with uniform distributions. The objectives vectors c and d are generated from the intervals $[0\ 1]$ and $[1\ 3]$, respectively. For Figures 3.1 and 3.2, the matrix $B = 0$, and the matrix M is generated with up to 2,000 nonzero entries and of the form:

$$M \equiv \begin{bmatrix} D_1 & E^T \\ -E & D_2 \end{bmatrix}, \tag{3.30}$$

where D_1 and D_2 are positive diagonal matrices of random order and with elements chosen from [0 2], and E is arbitrary with elements in [-1 1]. The vector q is randomly generated with elements in the interval [-20 -10]. Note that M is positive definite, albeit not symmetric. This property of M and the choice of $B = 0$ ensure LPCC feasibility, and thus optimality (because c and d are nonnegative and the variables are nonnegative). For Figure 3.3, $B \neq 0$ and the matrix M has no special structure but has only 10% density. The rest of the data A, f, q, and N are generated to ensure LPCC feasibility, and thus optimality. Details of the data generation and the resulting data can be found on the webpage http://www.rpi.edu/ mitchj/generators/lpcc/.

Figures 3.1, 3.2, and 3.3 detail the progress of the runs, showing in particular how LPCC_{ub} decreases with the number of iterations. The vertical axis refers to the LPCC objective values and the horizontal axis labels the number of iterations as defined in the opening paragraph of Section 3.4. The top value on the vertical axis is the LPCC objective value obtained at termination of the pre-processor with the LPCC feasibility recovery step. The bottom value is verifiably $\text{LPCC}_{\min}$. The vertical axis is scaled differently in each run with respect to the difference between the top and the bottom values. As comparison, the objective values obtained from FILTER (marked by the red square) and KNITRO (marked by the blue diamond) are also shown on the vertical axis; if the difference between the FILTER and KNITRO values in a run is within 1e-3, we only mark the KNITRO result (the exact values from these two solvers can be found in Tables 3.1, 3.2, and 3.3). The upper limit of the horizontal axis indicates the number of IPs needed to be solved in each run. Note that in some runs, a globally optimal solution might have been obtained in an earlier iteration without certification, and the algorithm needs more subsequent iterations to verify its global optimality. For example, in the fourth run of the right-hand column in Figure 3.1, a globally optimal solution is first obtained at iteration 2, but the certificate is established only after 23 more iterations. Other details about the figures are summarized in the remarks below the figures.

Corresponding to the problems in Figures 3.1, 3.2, and 3.3 respectively, Tables 3.1, 3.2, and 3.3 report more details about the runs, which are indexed by counting first row-wise and then column-wise in the figures (for example, the fourth run in Table 3.1 is the second row on the right column in Figure 3.1). In addition to the objective values obtained in our algorithm and from the NEOS solvers, these tables also report the numbers of IPs and LPs (excluding the $\lfloor m/3 \rfloor$ relaxed LPs solved in the pre-processor), solved in the solution process. These numbers, which are independent of the computational platform and machine, provide a good indicator of the efforts required by the algorithm in processing the LPCCs. We did not report computational times for two reasons: (i) the MATLAB results are computer dependent and the runs involve interfaces between MATLAB and CPLEX, and (ii) our runs are experimental and the coding is at an amateur level.

The computational results for the infeasible and unbounded LPCCs are reported in Table 3.4, which contains 3 sub-tables (a), (b), and (c). The first two sub-tables (a) and (b) pertain to feasible but unbounded LPCCs. For the unbounded problems, we set $B = 0$, q is arbitrary, and we generate A with a nonnegative column, M given by (3.30) and f such that $\{x \geq 0 : Ax \geq f\}$ is feasible. Problems in (a) and (b) have the same parameters except for the objective vector c and d and matrix A. For the problems in (a), we simply maximize one single x-variable whose A column is nonnegative. For the problems in (b), the objective vectors c and d are both negative; and the matrix A is the same as it is in group (a) except that a small number 0.005 is added to its nonnegative column (see the discussion in the first conclusion below for why this is done). The third sub-table (c) pertains to a class of infeasible LPCCs generated as follows: q, N, and M are all positive so that the only solution to the LCP: $0 \leq y \perp q + Nx + My \geq 0$ for $x \geq 0$ is $y = 0$; $Ax + By \geq f$ is feasible for some $(x, y) \geq 0$ with $y \neq 0$ but $Ax \geq f$ has no solution in $x \geq 0$.

To illustrate the effectiveness of the sparsification step, we generated some LPCCs with $n = m = k = 25$ and the same characteristics as the problems in Figure 3.3.

Table 3.5 reports the numbers of LPs and IPs that are needed to be solved in both runs with or without the sparsification step.

The main conclusions from the experiments are summarized below.

• The algorithm successfully terminates with the correct status of all the LPCCs reported. In fact, we have tested many more problems than those reported and obtained similar success. There are, nevertheless, a few instances where the LPCC are apparently unbounded but the algorithm fails to terminate after 6,000 iterations without the definitive conclusion, even though the LPCC objective is noticeably tending to $-\infty$. We cannot explain these exceptional cases which we suspect are due to round-off errors in the computations. This suspicion led us to add the small 0.005 in the unbounded set of runs reported above; with this small adjustment, the algorithm successfully terminated with the desired certificate of unboundedness.

• For the special LPCCs with $B = 0$, the results from the two NEOS algorithms, FILTER and KNITRO, are proved to be suboptimal in 2 out of the 20 runs (the first and fourth runs on the left column in Figure 3.1). In the other 18 runs, our algorithm is able to obtain an optimal solution with little computational effort (within 5 iterations), but requires significant additional computations to produce the desired certificate of global optimality. For the general LPCCs with $B \neq 0$, the objective values obtained from FILTER and KNITRO are suboptimal in 6 out of 10 runs. In the other 4 runs, only 5 iterations are needed to derive either a globally optimal solution or an LPCC feasible solution whose objective value is within 3% of the optimal value. These results confirm that the verification of global optimality is generally much more demanding than the computation of the solution without proof of optimality.

• Except for one problem (problem 7 in Table 3.3), the solutions obtained by the simple-cut pre-processor for all LPCCs with finite optima are within 5% of the globally optimal solutions. In fact, some of the solutions obtained from the pre-processing are immediately verified to be optimal. This suggests that very high-quality LPCC feasible solutions can be produced efficiently by solving a reasonable number of LPs.

• The sparsification procedure is quite effective; so is the LPCC feasibility recovery step. Indeed without the latter, there is a significant percentage of problems where the algorithm

#	LPCC_{lb} rxLPCC	preprocess	LPCC_{ub} preprocess	$\text{LPCC}_{\min}$	FILTER	KNITRO	LP	IP
1	1094.6041	1106.8297	1146.7550	1127.4885	1140.5614_{5}	1141.6696_{52}	396	18
2	1172.1830	1176.6893	1185.0192	1182.2146	1182.2145_{5}	1182.2147_{47}	57	1
3	820.2584	823.8912	823.9099	823.9055	823.9055_{10}	823.9058_{55}	14	1
4	796.9560	813.9752	840.4828	833.9718	833.9717_{6}	833.9718_{41}	611	22
5	841.1786	849.0122	850.2416	849.8451	849.8451_{5}	849.8452_{44}	66	1
6	924.7529	926.1028	926.5924	926.5000	926.5000_{5}	926.5000_{56}	21	1
7	1536.1748	1541.4464	1543.8863	1541.9443	1543.1950_{6}	1543.1951_{55}	35	1
8	1076.8760	1090.2155	1109.1441	1106.3617	1106.3616_{5}	1113.8938_{70}	363	25
9	1232.7912	1239.7156	1239.8283	1239.8283	1239.8284_{7}	1239.8285_{62}	10	1
10	1217.1191	1229.2734	1250.6693	1249.9884	1249.9884_{8}	1249.9886_{67}	832	46

Table 3.1: Special LPCCs with $B = 0$, $A \in \Re^{90\times 100}$, and 100 complementarities.

Remark: The first column "#" is the problem counter; the second column "LPCC_{lb}" contains the objective values of LP relaxations before and after the pre-processing. The column "LPCC_{ub}" reports the objective values of the LPCC feasible solutions. The right subcolumn contains the verifiably optimal $\text{LPCC}_{\min}$. The left subcolumn contains the values obtained after pre-processing with the LPCC feasibility recovery procedure. The objective values obtained from FILTER and KNITRO are reported in the next columns. (Note that these values are very comparable and practically optimal in all problems except #1 and 7 for both and 8 for KNITRO.) The total number of LPs solved (excluding the $\lfloor m/3 \rfloor$ relaxed LPs in the pre-processing step), and the number of IPs solved in the run are reported in the last two columns. At the suggestion of a referee, we also reported the number of "major iterations" in the two NEOS solvers; these are placed as subscripts in the objective values of the respective solvers. It should be noted that such iterations refer to different procedures in the two solvers.

fails to make progress after 3,000 iterations. With this step installed, all problems are resolved satisfactorily.

• While the numbers of IPs solved are quite reasonable in most cases, there are several runs where the numbers of relaxed LPs solved are unusually large, especially when the problem size increases. This suggests that stronger cuts are needed for both general LPCCs and for specialized problems arising from large-scale applications. The implementation of a dedicated solver for satisfiability problems, such as those described in [8, 40], could considerably improve the overall solution times of the LPCC algorithm. These refinements of the algorithm are presently being investigated.

#	LPCC_{lb} rxLPCC	LPCC_{lb} preprocess	LPCC_{ub} preprocess	LPCC_{ub} $\text{LPCC}_{\min}$	FILTER	KNITRO	LP	IP
1	2469.4400	2474.3166	2479.1835	2478.2254	2478.2256_{19}	2478.2264_{66}	125	1
2	3213.7176	3229.1930	3299.1115	3270.1842	3280.1865_{8}	3270.1844_{72}	4071	62
3	3639.4490	3651.5714	3671.6385	3660.5407	3660.5412_{42}	3660.5412_{79}	350	2
4	3127.3708	3140.3119	3265.7213	3176.4109	3176.4108_{11}	3176.4115_{69}	1249	15
5	2958.9147	2959.9381	2959.9498	2959.9498	2959.9495_{6}	2959.9529_{66}	5	1
6	2630.3282	2645.6771	2703.0018	2672.5706	2684.5288_{30}	2672.5710_{60}	4511	70
7	2616.9852	2617.2640	2617.2640	2617.2640	2617.2638_{14}	2617.2673_{65}	0	0
8	2766.9544	2770.1510	2771.3315	2771.2374	2771.2372_{27}	2771.2379_{70}	26	1
9	2842.4480	2846.7174	2847.9806	2847.6923	2847.6926_{7}	2847.6929_{48}	319	2
10	3207.6861	3220.3810	3235.4082	3230.9893	3230.9896_{6}	3230.9897_{66}	1569	16

Table 3.2: Special LPCCs with $B = 0$, $A \in \Re^{200\times 300}$, and 300 complementarities.

Remark: The explanation of this table is the same as Table 1. Note that in the problem 7, the solution obtained after the pre-processing step is immediately verified to be globally optimal. For these runs, the KNITRO solutions are practically optimal in all cases; but the FILTER solution in problem #2 is noticeably suboptimal.

#	LPCC_{lb} rxLPCC	LPCC_{lb} preprocess	LPCC_{ub} preprocess	LPCC_{ub} $\text{LPCC}_{\min}$	FILTER	KNITRO	LP	IP
1	28.7739	29.0318	29.0502	29.0501	29.0501_{8}	30.0155_{32}	21	2
2	36.1885	36.8258	39.1063	37.5509	37.5509_{7}	37.5510_{25}	229	9
3	33.8630	34.4988	39.1285	37.0022	38.3216_{7}	38.7521_{28}	4842	696
4	33.7618	34.1479	34.3034	34.2228	34.6057_{5}	34.2398_{54}	102	7
5	21.4187	21.9246	22.9642	22.2835	22.2945_{5}	22.2837_{35}	209	24
6	29.8919	29.9681	30.1085	30.0829	30.0829_{6}	30.0830_{26}	108	13
7	37.6712	37.9972	38.0405	38.0405	38.0419_{6}	38.0419_{29}	92	7
8	20.8210	21.4586	27.9618	22.3969	22.7453_{7}	22.4164_{37}	187	21
9	39.0227	39.4792	40.7839	40.3380	44.7872_{8}	44.3173_{26}	321	14
10	40.0135	40.7994	41.6865	41.3957	41.5810_{5}	41.5810_{37}	190	19

Table 3.3: General LPCCs with $B \neq 0$, $A \in \Re^{55\times 50}$, and 50 complementarities.
Remark: For these runs, there are more instances where the two NEOS solutions are noticeably suboptimal.

Prob	# iters	# cuts	# LPs	# iters	# cuts	# LPs	# iters	# cuts	# LPs
1	50	47	195	4	3	9	14	14	28
2	6	4	14	5	4	12	2	2	4
3	1081	828	2604	2	1	5	38	38	76
4	166	144	424	42	39	120	7	7	14
5	436	305	991	735	621	1860	47	49	100
6	18	17	54	498	379	1125	48	48	96
7	3	4	11	352	127	663	20	20	40
8	426	356	1191	489	373	1158	13	13	26
9	9	9	26	5	4	12	50	50	100
10	4	3	11	9	7	22	6	6	12
		(a)			(b)			(c)	

Table 3.4: Infeasible and unbounded LPCCs with 50 complementarities.

iters = number of returns to Step 1 = number of IPs solved
cuts = number of satisfiability constraints in $\mathcal{Z}_{\text{work}}$ at termination
LPs = number of LPs solved, excluding the $\lfloor m/3 \rfloor$ relaxed LPs in the pre-processing step

	A		B	
Prob	# LPs	# IPs	# LPs	# IPs
1	122	122	61	18
2	17	17	33	11
3	7	7	51	9
4	16	16	41	12
5	280	280	70	21
6	598	598	85	23
7	195	195	90	26
8	65	65	43	10
9	9	9	41	9
10	8	8	33	8

Table 3.5: General LPCCs with $B \neq 0$, $A \in \Re^{25\times 25}$, and 25 complementarities
column A = number of IPs or LPs solved in the run without sparsification
column B = number of IPs or LPs solved in the run with sparsification.

Remark: In column A, the number of IPs solved in the run is equal to the number of solved LPs. Except for the problems 3, 9 and 10, the B approach (with sparsification step implemented) is doing much better than the A approach. Especially for problems 1, 5–8, the numbers of IPs and LPs are dramatically reduced. For the remaining problems, the computational effort with sparsification is at least comparable to, if not better than, the approach without sparsification. With the number of complementarities in the LPCCs grows, we expect more computational savings with the sparsification step implemented.

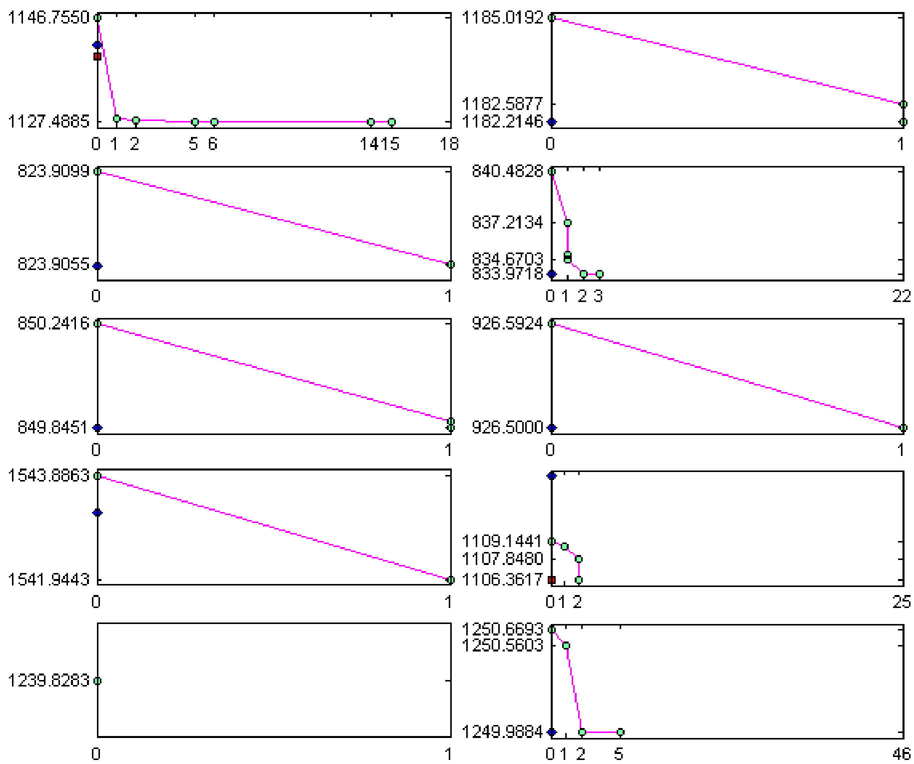

Figure 3.1: Special LPCCs with $B = 0$, $A \in \Re^{90\times 100}$, and 100 complementarities.

Remark: Each circle signifies that a better feasible LPCC solution is found. The circle's horizontal coordinate indicates the iteration where LPCC_{ub} is updated; its vertical coordinate gives the value of updated LPCC_{ub}, (we omitted some values if they are not significantly improved). Note that it is possible for LPCC_{ub} to improve within one iteration by the sparsification step; see the example in Subsection 3.4.1 and also the top run in the right column. In the fifth run in the left column, both of the FILTER and KNITRO results coincide with $\text{LPCC}_{\min}$, which is obtained after pre-processing and verified to be optimal after 1 iteration.

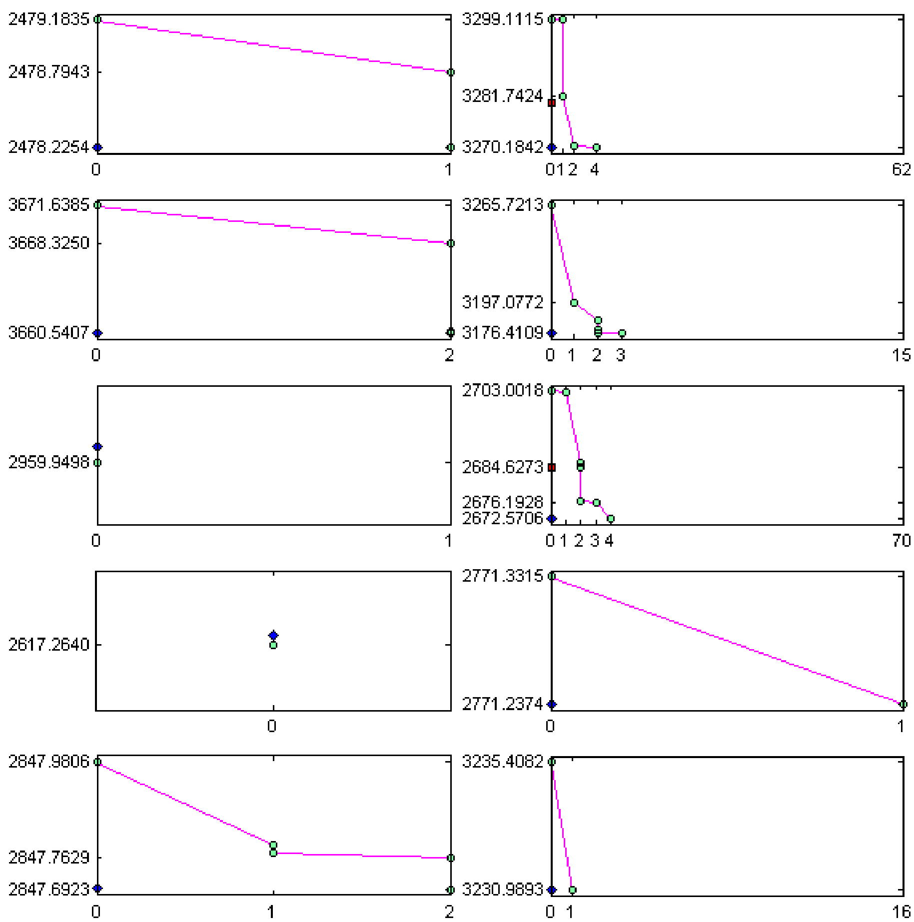

Figure 3.2: Special LPCCs with $B = 0$, $A \in \Re^{200\times300}$, and 300 complementarities.

Remark: The explanation for the figure is similar to that of Figure 1. Note that in the third and fourth runs in the left column, LPCC_{ub} is obtained right after preprocessing. In the third run, the solution's global optimality is verified after 1 iteration; while in the fourth run, the solution is immediately verified to be globally optimal (the difference between the upper and lower bound of the LPCC is within 1e-6).

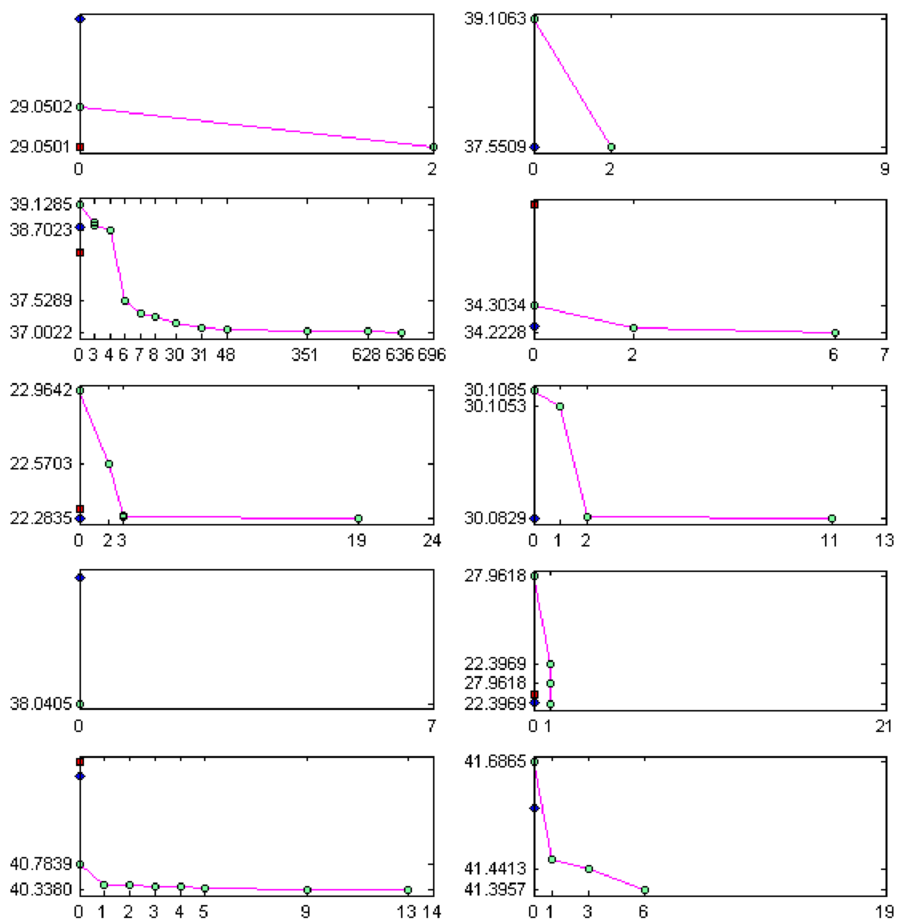

Figure 3.3: General LPCCs with $B \neq 0$, $A \in \Re^{55\times 50}$, and 50 complementarities.

CHAPTER 4
GLOBALLY RESOLVING THE INDEFINITE QPS

In this chapter, we will present an LPCC approach that is able to determine in finite time whether a given QP has an unbounded objective value on its feasible set, or compute a global optimal solution of the QP if such a solution exists. The task can be divided into two steps. The first step is to solve an LPCC whose resolution confirms whether or not the original QP is bounded below on its feasible set, and compute a feasible ray on which the quadratic objective goes to infinity if such a ray exists. If it is confirmed that this QP attains a finite optimal solution, another LPCC as an equivalent reformulation of the QP based on the first order KKT conditions is resolved to identify this optimal solution. These LPCCs can be resolved by the mixed integer-programming based, finitely terminating algorithm presented in Chapter 3. As an enhancement of the algorithm, a new kind of valid cut can be derived from the second-order conditions of the QP and the special structure of the formulated LPCC.

The organization of this chapter is as follows. In Section 4.1, we will have a preliminary discussion by showing some well-known facts of a general quadratic program. In Section 4.2, we will present the formulation of the LPCC whose global resolution determines the unboundedness of the QP, and provide the proof to validate this LPCC approach. Section 4.3 is focused on the specialization of the algorithm for resolving LPCCs to the QPs with finite optima. Section 4.4 introduces 3 classes of indefinite QPs that we use to illustrate the developed methodology. The numerical results are presented in Section 4.5 with a discussion about these results.

4.1 Preliminary Discussion

Consider the quadratic program:

$$\begin{aligned} \underset{x \in \Re^n}{\text{minimize}} \quad & q(x) \equiv \tfrac{1}{2} x^T Q x + c^T x \\ \text{subject to} \quad & Ax \le b, \end{aligned} \tag{4.1}$$

where Q is a symmetric, but not necessarily positive semidefinite, matrix of order n, A is an $m \times n$ matrix, and c and b are n- and m-vectors respectively. The feasibility of the above QP can be easily checked by solving a linear program. Thus we assume, without any loss of generality, that the set $\{x : Ax \leq b\}$, denoted as X, is a feasible set. Furthermore, we assume that the recession cone of X: $\mathcal{D} \equiv \{d \in \Re^n : Ad \leq 0\}$, is a subset of the nonnegative orthant $\Re^n_+$. This assumption will not cause any loss of generality, since (4.1) is obviously equivalent to the following problem:

$$
\begin{array}{ll}
\underset{x^{\pm} \in \Re^{2n}}{\text{minimize}} & \frac{1}{2}(x^+ - x^-)^T Q (x^+ - x^-) + c^T (x^+ - x^-) \\
\text{subject to} & A(x^+ - x^-) \leq b \\
\text{and} & x^{\pm} \geq 0.
\end{array}
$$

As a result of the previous assumption, we may truncate the recession cone into compact subsets with the addition of the single constraint $\mathbf{1}_n^T d \leq \rho$, where ρ is a positive scalar and $\mathbf{1}_n$ is the n-vector of all ones. A vector of the form $\{x + \tau d : \tau \geq 0\}$, where $(x, d) \in X \times \mathcal{D}$, is a feasible ray of X.

By denoting ξ as the dual variables associated with the constraints in the primal QP (4.1), the Karush-Kuhn-Tucker (KKT) conditions are stated as:

$$
\begin{array}{rcl}
0 & = & c + Qx + A^T \xi \\
0 & \leq & \xi \perp b - Ax \geq 0.
\end{array}
\tag{4.2}
$$

If there exists a pair (x, ξ) satisfying the KKT conditions (4.2), we call the vector $x \in X$ a KKT point, or equivalently a stationary point. The quadratic objective value of the QP (4.1) on the set of the stationary points becomes:

$$
\frac{1}{2} x^T Q x + c^T x = \frac{1}{2} c^T x - \frac{1}{2} b^T \xi
$$

Especially, for a pair (x, ξ) satisfying the KKT conditions (4.2), we define the following index sets for reference.

$$\begin{aligned}
\alpha(x,\xi) &\equiv \{\, j \,:\, b_j - A_{j\bullet}x \,=\, 0 \,<\, \xi_j \,\} \\
\beta(x,\xi) &\equiv \{\, j \,:\, b_j - A_{j\bullet}x \,=\, 0 \,=\, \xi_j \,\} \\
\gamma(x,\xi) &\equiv \{\, j \,:\, b_j - A_{j\bullet}x \,>\, 0 \,=\, \xi_j \,\}
\end{aligned}$$

By denoting $\mathcal{T}(x;X)$ as the tangent cone of the feasible set X at the point x, we have $\mathcal{T}(x;X) = \{d \in \Re^n : A_{i\bullet}d \leq 0 \;\forall\, i \in \alpha(x,\xi) \cup \beta(x,\xi)\}$. The critical cone of X at $x \in X$ is defined as $\mathcal{C}_{\rm qp}(x) \equiv \mathcal{T}(X;x) \cap (c+Qx)^{\perp}$, where $v^{\perp}$ denotes the linear subspace of vectors orthogonal to v. If x is a KKT point with a multiplier ξ satisfying the conditions (4.2), the critical cone $\mathcal{C}_{\rm qp}(x)$ can be represented as:

$$\mathcal{C}_{\rm qp}(x) \,=\, \left\{ \begin{array}{rl} v \,\in\, \Re^n \,:\, & A_{j\bullet}v \,=\, 0, \quad \forall\, j \,\in\, \alpha(x,\xi) \\ & A_{j\bullet}v \,\leq\, 0, \quad \forall\, j \,\in\, \beta(x,\xi) \end{array} \right\}.$$

As a result of the above representation, the lineality space of $\mathcal{C}_{\rm qp}(x)$ can be written as

$$\mathcal{C}_{\rm qp}(x) \,\cap\, (\,-\mathcal{C}_{\rm qp}(x)\,) \,=\, \bigcap_{i \in \alpha(x,\xi) \cup \beta(x,\xi)} \{\, v \,\in\, \Re^n \,:\, A_{i\bullet}v \,=\, 0 \,\}\,.$$

We recall that a matrix M is copositive on a cone C if $x^TMx \geq 0$ for all $x \in C$; M is strictly copositive on C if $x^TMx > 0$ for all nonzero $x \in C$.

Proposition 11 below is a summary of various known facts about the QP (4.1). Proofs of these results can be found in the cited references.

Proposition 11. Suppose that the QP (4.1) is feasible.

(a) [54] A feasible vector $x \in X$ is a (strict) local minimum of (4.1) if and only if x is a KKT point and Q is (strictly) copositive on $\mathcal{C}_{\rm qp}(x)$.

(b) [23] The QP (4.1) attains a global minimum solution if and only if its objective function is bounded below on X, or equivalently, on the feasible rays of X; furthermore, this holds if and only if (a) Q is copositive on $\mathcal{D}$, and (b) $(c+Qx)^Td \geq 0$ for all $(x,d) \in X \times \mathcal{D}$ satisfying $d^TQd = 0$.

(c) [53] The quadratic objective function attains finitely many values on the set of stationary points of (4.1).

(d) [32] If the QP (4.1) has a finite optimal solution, then the minimum objective value is equal to the minimum stationary value. □

Part (a) provides necessary and sufficient conditions for a feasible solution to be a (strict) local minimum of the QP (4.1); part (b) provides necessary and sufficient conditions for the QP (4.1) to attain a finite optimal solution; part (c) asserts that a quadratic program, which is known in advance to be bounded below on its feasible region, has a finite number of stationary values, which are the objective values obtained on the set of stationary points; part (d) asserts that the minimum of these stationary values yields the optimal objective value of the QP (4.1). Based on these results, the optimal solution of the QP (4.1) that is optimally solvable, can be computed by solving the following LPCC.

$$\begin{array}{ll} \underset{(x,\xi)\in\Re^{n+m}}{\text{minimize}} & c^T x - b^T \xi \\ \text{subject to} & 0 \,=\, c + Qx + A^T\xi \\ & 0 \,\leq\, \xi \,\perp\, b - Ax \,\geq\, 0. \end{array} \tag{4.3}$$

Unfortunately, the LPCC (4.3) alone doesn't provide any information about the boundedness of the original QP (4.1). As a matter of fact, the feasible ray of set X, on which the objective of QP (4.1) is unbounded below, doesn't necessarily emanate from any of the stationary points or their convex hull. The following QP is a simple example illustrating this point.

$$\begin{array}{ll} \underset{(x_1,x_2)\in\Re^2}{\text{minimize}} & (\,x_1 - 1\,)\,(\,x_2 - 1\,) \\ \text{subject to} & x_1, x_2 \,\geq 0. \end{array} \tag{4.4}$$

This QP has a unique KKT point (1,1). The recession cone of the feasible region is the nonnegative orthant $\Re^2_+$. Although the objective is unbounded below on two rays, (0,1) and (1,0), emanating from the origin, yet the same function is bounded below on any feasible ray starting at the stationary point.

One noteworthy property about the QP is that: if $d \in \mathcal{D}$ is such that $d^TQd > (<)0$, then for any vector x, $q(x + \tau d) \to \infty(-\infty)$ as $\tau \to \infty$. Thus as far as the boundedness of the QP is concerned, we are more interested about the rays where $d^TQd = 0$. We denote the set of these feasible rays as $\mathcal{D}_0$ and call them the *essential recession directions*. Also denote $\mathcal{S}$ as the convex hull of the stationary points. The following result states that on those *essential recession directions* emanating from the convex hull of the stationary points, the objective of the QP is always bounded below.

Proposition 12. Given a quadratic program (4.1), for any $(x, d) \in \mathcal{S} \times \mathcal{D}_0$,

$$\liminf_{\tau \to \infty} q(x + \tau d) > -\infty.$$

Proof. For any stationary point $\bar{x}$, we have $C + Q\bar{x} = -A^T \xi$; for any recession direction $d \in \mathcal{D}$, we have $Ad \leq 0$. Thus $(c + Q\bar{x})^T d \geq 0$ holds for all stationary points and all feasible rays, it follows that $(c + Qx)^T d \geq 0$ for all $(x, d) \in \mathcal{S} \times \mathcal{D}_0$. Hence, we have $q(x + \tau d) = q(x) + \tau (c + Qx)^T d + \frac{1}{2}\tau^2 d^T Q d \geq q(x)$ for all $\tau \geq 0$. $\square$

Therefore, we can't simply focus on the set of the stationary points or their convex combination to check the unboundedness of a given QP. To identify the unboundedness, we need to broaden our search outside of the convex hull of the stationary points. Recognizing this fact, we formulated the following problem as the truncated QP:

$$\begin{array}{lll} \underset{x \in \Re^n}{\text{minimize}} & q(x) \equiv \frac{1}{2} x^T Q x + c^T x & \\ \text{subject to} & Ax \leq b & \qquad (4.5) \\ \text{and} & \mathbf{1}_n^T x \leq \rho, & \end{array}$$

which must have a nonempty, bounded feasible set for any sufficiently large value of $\rho > 0$, due to the preassumption that the recession cone $\mathcal{D} \subseteq \Re^n_+$. A finite optimal solution of (4.5), namely x^ρ, must exist and can be computed, along with multipliers (ξ^ρ, t_ρ), by solving the LPCC:

$$\begin{array}{ll} \underset{(x,\xi,t) \in \Re^{n+m+1}}{\text{minimize}} & c^T x - b^T \xi - t\,\rho \\ \text{subject to} & 0 = c + Qx + A^T \xi + t\,\mathbf{1}_n \\ & 0 \leq \xi \perp b - Ax \geq 0 \\ & 0 \leq t \perp \rho - \mathbf{1}_n^T x \geq 0. \end{array} \qquad (4.6)$$

Motivated by the part (b) of Proposition 11, we formulate another QP to check the copositivity of matrix Q on the recession cone $\mathcal{D}$:

$$\begin{array}{ll} \underset{d \in \Re^n}{\text{minimize}} & \frac{1}{2}\, d^T Q d \\ \text{subject to} & Ad \,\leq\, 0 \\ \text{and} & \mathbf{1}_n^T d \,=\, 1, \end{array} \tag{4.7}$$

in which the recession cone $\mathcal{D} = \{d \,:\, Ad \,\leq\, 0\}$ of the original QP (4.1) is truncated by the scaler 1. The obtained problem (4.7) has a bounded feasible region; thus a finite optimal solution must exist and can be computed by solving the LPCC:

$$\begin{array}{ll} \underset{(d,\lambda,s) \in \Re^{n+m+1}}{\text{minimize}} & -s \\ \text{subject to} & 0 \,=\, Qd + A^T \lambda + s\, \mathbf{1}_n \\ & 0 \,\leq\, \lambda \,\perp\, -Ad \,\geq\, 0 \\ & s \text{ free}, \quad 1 - \mathbf{1}_n^T d \,=\, 0. \end{array} \tag{4.8}$$

It follows that the QP (4.1) is unbounded on one of its feasible rays if the LPCC (4.8) has a solution that yields a negative objective value. The copositivity of Q on the recession cone $\mathcal{D}$ provides a necessary condition for the existence of an optimal solution to the QP (4.1).

4.2 The LPCC Formulation

The unboundedness of the QP (4.1) can be resolved by combining the two LPCCs (4.6) and (4.8) into one LPCC, which is formulated as:

$$\begin{array}{ll} \underset{(x,d,\xi,\lambda,\mu,t,s)\in\Re^{2n+3m+2}}{\text{minimize}} & -t \\ \text{subject to} & 0 \,=\, c + Qx + A^T\xi + t\,\mathbf{1}_n \\ & 0 \,=\, Qd + A^T\lambda - A^T\mu + s\,\mathbf{1}_n \\ & 0 \,\leq\, \xi \,\perp\, b - Ax \,\geq\, 0 \\ & 0 \,\leq\, \mu \,\perp\, b - Ax \,\geq\, 0 \\ & 0 \,\leq\, \lambda \,\perp\, -Ad \,\geq\, 0 \\ & 0 \,\leq\, \xi \,\perp\, -Ad \,\geq\, 0 \\ & 0 \,\leq\, \mu \,\perp\, -Ad \,\geq\, 0 \\ & 0 \,\leq\, s, \quad \mathbf{1}_n^T d \,\geq\, 1. \end{array} \tag{4.9}$$

The key thing in such a formulation is that the parameter ρ in the LPCC (4.6) can be treated implicitly. The global resolution of this complete LPCC (4.9) provides a certificate of (un)boundedness of the original QP based on the following theorem.

Theorem 13. Suppose the QP (4.1) is feasible. This QP is unbounded below if and only if the LPCC (4.9) has a feasible solution with a negative objective value.

Proof. The 'if' part can be easily proved. Suppose that the LPCC has a feasible solution $(x, d, \xi, \lambda, \mu, t, s)$ with $t > 0$, then it follows that:

$$0 \,=\, d^T(\,Qd + A^T\lambda - A^T\mu + s\,\mathbf{1}_n\,) \,=\, d^TQd + s\mathbf{1}_n^Td,$$

which implies that $d^TQd \,\leq\, 0$, since $s \geq 0$ and $\mathbf{1}_n^Td \geq 1$. Moreover,

$$0 \,=\, d^T(\,c + Qx + A^T\xi + t\,\mathbf{1}_n\,) \,=\, d^T(\,c + Qx\,) + t\,\mathbf{1}_n^Td,$$

which implies that $d^T(c + Qx) \,=\, -t\,\mathbf{1}_n^Td \,<\, 0$. Consequently, we have $q(x + \tau d) \,=\, q(x) + \tau d^T(c + Qx) + \frac{1}{2}\tau^2 d^TQd \,\rightarrow\, -\infty$ as $\tau \,\rightarrow\, \infty$. This shows that the QP (4.1) is unbounded below on the ray $d \in \mathcal{D}$ emanating from the point x feasible to the QP (4.1).

Conversely, suppose the QP (4.1) is unbounded below on the feasible set $\{x : Ax \leq b\}$. Let $\{\rho_k\}$ be a sequence of escalating positive scalars with $\lim_{k\to\infty} \rho_k = \infty$, and x^k be the optimal solution of the truncated QP (4.5) with respect to each parameter ρ_k. It follows that:

$$\lim_{k\to\infty} q(x^k) = -\infty.$$

Denote (ξ^k, t_k) as the KKT multiplier with respect to x^k such that

$$\begin{array}{rcll} (\, x^k, \xi^k, t_k \,) & \in & \underset{(x,\xi,t)\in\Re^{n+m+1}}{\text{argmin}} & c^T x - b^T \xi - t\,\rho_k \\ & & \text{subject to} & 0 = c + Qx + A^T \xi + t\,\mathbf{1}_n \\ & & & 0 \leq \xi \perp b - Ax \geq 0 \\ & & \text{and} & 0 \leq t \perp \rho_k - \mathbf{1}_n^T x \geq 0. \end{array}$$

From the constraints of the above problem, we know that when $t_k = 0$, the pair $(\, x^k, \xi^k \,)$ satisfies the KKT conditions (4.2) of the original QP (4.1). Part (c) of Proposition (11) asserts that the function $q(x)$ attains finitely many values on the set of the QP's stationary points. It follows that, except for finitely many k's, we must have $t_k > 0$. Thus we may assume that $t_k > 0$ for all k without any loss of generality, and this implies that $\mathbf{1}_n^T x^k = \rho^k$ for all k. Thus the sequence $\{x^k\}$ must be unbounded. Let α be the index set of the active constraints where $(Ax^k - b)_\alpha = 0$ for infinitely many k, and $\bar{\alpha}$ be the complement of set α in $\{1, \ldots, m\}$. By working with the corresponding subsequence of $\{x^k\}$, we can assume without any loss of generality that

$$x^k \in \widehat{X} \equiv \{\, x \in X \,:\, (\, Ax - b\,)_\alpha = 0 \,\} \text{ and } (\, Ax^k - b\,)_{\bar{\alpha}} < 0, \quad \forall\, k.$$

Apparently, $\xi^k_{\bar{\alpha}} = 0$ for all k by the complementarity. Let $\widehat{X}^e$ be the convex hull of the extreme points of the set $\widehat{X}$ and $\widehat{\mathcal{D}}$ be the recession cone of $\widehat{X}$; it follows that

$$\widehat{D} = \{\, d \in \mathcal{D} \,:\, (\, Ad\,)_\alpha = 0 \,\} \subset \Re^n_+.$$

For each k, we may write

$$x^k \equiv \widehat{x}^k + \tau_k \, d^k,$$

for some $\widehat{x}^k \in \widehat{X}^e$, $\tau_k > 0$, and $d^k \in \widehat{\mathcal{D}}$ such that $\mathbf{1}_n^T d^k = 1$. Since the sequence $\{x^k\}$ is unbounded and each d^k has unit norm, we must have $\lim_{k \to \infty} \tau_k = \infty$. Without any loss of generality, we can assume that the sequence of $\{d^k\}$ converges to d^∞ as $k \to \infty$. d^∞ must be an element of $\widehat{\mathcal{D}}$ satisfying $\mathbf{1}_n^T d^\infty = 1$. Based on the fact that

$$q(x^k) = q(\widehat{x}^k) + \tau_k \, (c + Q\widehat{x}^k)^T d^k + \tfrac{1}{2}\tau_k^2 (d^k)^T Q d^k,$$

in which $q(x^k) \to -\infty$ and $\tau_k \to \infty$, we have $(d^\infty)^T Q d^\infty \leq 0$. Hence d^∞ must be feasible to the following QP:

$$\begin{array}{ll}
\underset{d}{\text{minimize}} & \frac{1}{2} d^T Q d \\
\text{subject to} & d \in \widehat{\mathcal{D}} = \{ d : Ad \leq 0, \, (Ad)_\alpha \geq 0 \} \\
\text{and} & \mathbf{1}^T d \leq 1.
\end{array} \tag{4.10}$$

Suppose that $\widehat{d}$ is the optimal solution for (4.10) satisfying $\widehat{d} \neq 0$ (otherwise, the problem (4.10) attains global optimality at 0; thus we can use d^∞ to replace $\widehat{d}$). Denote the tuple $(\widehat{\lambda}, \widehat{\mu}, \widehat{s})$ with $\widehat{\mu}_{\bar{\alpha}} = 0$ as the corresponding multiplier, which, together with $\widehat{d}$, satisfies the following KKT conditions of (4.10):

$$\begin{aligned}
0 &= Qd + A^T\lambda - A^T\mu + s\mathbf{1}_n \\
0 &\leq \lambda \perp -Ad \geq 0 \\
0 &\leq \mu \perp -Ad \geq 0 \\
0 &\leq s \perp 1 - \mathbf{1}_n^T d \geq 0.
\end{aligned}$$

Based on the definitions of α and $\bar{\alpha}$, we already have $\xi^k \perp -A\widehat{d}$ and $\widehat{\mu} \perp b - Ax^k$. Consequently, we obtain a tuple $\left(x^k, \sigma\widehat{d}, \xi^k, \sigma\widehat{\lambda}, \sigma\widehat{\mu}, t_k, \sigma\widehat{s}\right)$, where $\sigma \equiv 1/\mathbf{1}_n^T\widehat{d}$, feasible to the LPCC (4.9) with $t_k > 0$. This completes the "only if" part of the statement. $\square$

Notice that in the above proof, we have worked with the cone $\widehat{\mathcal{D}}$ instead of the whole recession cone $\mathcal{D}$. The variable μ has been introduced to restrict the recession directions within $\widehat{\mathcal{D}}$. The LPCC (4.9) is a complete formulation to provide a certificate of unboundedness of the QP (4.1), without any prior knowledge of the QP. If the copositivity of the matrix Q on the recession cone $\mathcal{D}$ is confirmed, we can drop the variable μ and use a simplified formulation of LPCC to determine the unboundedness.

Corollary 14. Suppose the QP (4.1) is feasible and Q is copositive on $\mathcal{D}$. This QP is unbounded below if and only if the LPCC:

$$\begin{array}{ll} \underset{(x,d,\xi,\lambda,t)}{\text{minimize}} & -t \\ \text{subject to} & 0 \;=\; c + Qx + A^T\xi + t\,\mathbf{1}_n \\ & 0 \;=\; Qd + A^T\lambda \\ & 0 \;\leq\; \xi \;\perp\; b - Ax \;\geq\; 0 \\ & 0 \;\leq\; \lambda \;\perp\; -Ad \;\geq\; 0 \\ & 0 \;\leq\; \xi \;\perp\; -Ad \;\geq\; 0 \\ & 1 \;\leq\; \mathbf{1}_n^T d \end{array} \tag{4.11}$$

has a feasible solution with a negative objective value.

Proof. Notice that every feasible solution of (4.11), together with $\mu = 0$ and $s = 0$, is also feasible for the LPCC (4.9). This completes the 'if' part of the corollary. Conversely, under the copositivity assumption of the matrix Q on $\mathcal{D}$, the recession direction d^∞ defined in the proof of Theorem 13 must be an optimal solution to the following QP:

$$\begin{array}{ll} \underset{d}{\text{minimize}} & \frac{1}{2}\, d^T Q d \\ \text{subject to} & Ad \;\leq\; 0. \end{array}$$

By necessary scaling, we can prove the 'only if' part similarly to the proof of Theorem 13. $\square$

4.3 Specialization to Solvable QPs

As we illustrated in Section 4.2, the task of globally resolving a general QP (4.1) without any preassumption of boundedness can be divided into two LPCCs: the first

LPCC (4.9) determines whether the given QP is unbounded on its feasible region and computes a feasible ray on which the objective is unbounded if such a ray exists; the second LPCC (4.3) computes a globally optimal solution if it exists. Nevertheless, both of the LPCCs can be accomplished by a parameter-free, mixed-integer programming based algorithm which has been presented in Chapter 3. Following the terminology used in Chapter 3, we summarize the key steps implemented in the algorithm as follows.

Sketch of an algorithm

Step 0. Generate some initial cuts by a pre-processing procedure.

Step 1. Solve a satisfiability feasibility system to determine a binary vector z and let $\alpha \equiv \text{supp}(z)$.

Step 2. Solve the homogeneous LP (3.10). If $\varphi_0(z) = \infty$, then a ray cut is obtained. Otherwise, solve either the primal LP (3.2) or its dual (3.9) to obtain either a point cut or an unboundedness certificate for the LPCC.

Step 3. Apply a problem-specific procedure to sparsify the obtained cut(s), by solving tight LP relaxations of the LPCC restricted by the sparsified cut under testing. Add the sparsified cuts to update the satisfiability system. Return to Step 1.

The details of the algorithm sketched above lie in the generation of the initial cuts in the pre-processing procedure and the sparsification step. In this section, we are restricting our discussion to the QP (4.1) in a general form which is assumed to attain a finite optimal solution. Thus, the QP (4.1) can be resolved by solving its equivalent LPCC problem (4.3), whose conceptual MIP formulation is:

$$\begin{array}{ll} \underset{(x,\xi,z)}{\text{minimize}} & c^T x - b^T \xi \\ \text{subject to} & 0 \,=\, c + Qx + A^T \xi \\ & 0 \,\leq\, b - Ax \,\leq\, \theta\, z \\ & 0 \,\leq\, \xi \,\leq\, \theta\,(\,\mathbf{1}_m - z\,) \\ \text{and} & z \,\in\, \{\,0, 1\,\}^m. \end{array} \tag{4.12}$$

In what follows, we will present several key procedures that can be implemented to find an optimal solution of a solvable QP (4.1). The specialization of these procedures to each different type of indefinite QPs will be discussed in Subsection 4.4.1 and 4.4.2. In Subsection 4.4.3, we will briefly mention a nonnegatively constrained copositive QP that is not necessarily bounded.

4.3.1 Valid cuts from second-order necessary conditions

The second-order necessary optimality condition for the QP (4.1) stipulates that if x is a local minimum, then the matrix Q must be copositive on the critical cone $\mathcal{C}_{\rm qp}(x)$. Consequently, we have the following corollary.

Proposition 15. If x is a local minimum of the QP (4.1), then Q is positive semidefinite on the lineality space of $\mathcal{C}_{\rm qp}(x)$. $\square$

Motivated by Proposition 15, we can generate some satisfiability constraints in the pre-processing procedure and use them as valid cuts for the MIP (4.12). To introduce these inequalities, we define the family of index sets:

$$\mathcal{J} \equiv \{ J \subseteq \{1, \cdots, m\} : Q \text{ is not positive definite on the kernel of the matrix } A_{J\bullet} \}$$

and the set:

$$\mathcal{Z}_2 \equiv \left\{ z \in \mathcal{Z} : \sum_{j \notin J} (1 - z_j) \geq 1, \quad \forall J \in \mathcal{J} \right\}.$$

We call each inequality in the above set $\mathcal{Z}_2$ corresponding to a $J \in \mathcal{J}$ a *2nd-order cut* of the mixed IP (4.12). The proposition below asserts that the constraints contained in $\mathcal{Z}_2$ are valid cuts to the MIP (4.12). In other words, if the QP (4.1) attains a finite optimal solution, then there exists at least one binary vector corresponding to this optimal solution, such that it is feasible to $\mathcal{Z}_2$. In what follows, we denote $\text{QP}_{\min}$ as the optimal objective value of the QP (4.1).

Proposition 16. If the QP (4.1) has a finite optimal solution, then $\text{QP}_{\min} = \min_{z \in \mathcal{Z}_2} \varphi(z)$.

Proof. It is obviously true that $\text{QP}_{\min} = \min_{z \in \mathcal{Z}} \varphi(z) \leq \min_{z \in \mathcal{Z}_2} \varphi(z)$, since $\mathcal{Z}_2$ is a subset of $\mathcal{Z}$. Hence, it suffices to just show $\text{QP}_{\min} \geq \min_{z \in \mathcal{Z}_2} \varphi(z)$; or equivalently, it suffices to identify a binary vector $z \in \mathcal{Z}_2$ such that $\text{QP}_{\min} = \varphi(z)$. For this purpose, we denote x^* as an optimal solution of (4.1) with ξ^* being the associated KKT multiplier. Choose a binary vector $z^0 \in \mathcal{Z}$ such that $\mathrm{supp}(z^0) \equiv \{ i : (b - Ax^*)_i > 0 \} \equiv \alpha_0$. Let $\bar{\alpha}_0$ be the complement of α_0 in $\{1, \cdots, m\}$. The pair (x^*, ξ^*) must be an optimal solution to the LP piece corresponding to the index set α_0. It follows that $\mathrm{QP}_{\min} = \varphi(z^0)$, where

$$\begin{aligned} \varphi(z^0) \;=\; & \underset{(x,\xi) \in \Re^{n+m}}{\text{minimize}} \quad c^T x - b^T \xi \\ & \text{subject to} \quad 0 \;=\; c + Qx + A^T \xi \\ & \qquad\qquad\quad\; 0 \;=\; (\, b - Ax \,)_{\bar{\alpha}_0} \\ & \qquad\qquad\quad\; 0 \;\leq\; (\, b - Ax \,)_{\alpha_0} \\ & \qquad\qquad\quad\; 0 \;=\; \xi_{\alpha_0}, \quad \text{and} \quad 0 \;\leq\; \xi_{\bar{\alpha}_0}. \end{aligned}$$

Suppose that $\sum_{j \notin J_0} (1 - z^0_j) = 0$ for some index set $J_0 \in \mathcal{J}$; or equivalently, $z^0_j = 1$ for all $j \notin J_0$. It follows from the MIP (4.12) that $\xi^*_j = 0$ for all $j \notin J_0$. If $(b - Ax^*)_{\widehat{j}} = 0$ for some index $\widehat{j} \notin J_0$, by defining an alternative binary vector z^* where $z^*_k = z^0_k$ for all $k \neq \widehat{j}$ and $z^*_{\widehat{j}} = 0$, we still have $\varphi(z^*) = \mathrm{QP}_{\min}$ with $z^* \in \mathcal{Z}_2$. Thus, without loss of generality, we may assume that $(b - Ax^*)_j > 0$ for all $j \notin J_0$. Since $J_0 \in \mathcal{J}$, there exists a vector d with at least one nonzero component satisfying $A_{j\bullet} d = 0$ for all $j \in J_0$ and $d^T Q d \leq 0$. It then follows that $x^* + \tau d$ remains feasible to the QP (4.1) for all $\tau > 0$ sufficiently small; moreover, with $\tau > 0$ properly chosen, $b_j = A_{j\bullet}(x^* + \tau d)$ for at least one $j \notin J_0$. By multiplying d with both sides of the equation $c + Qx^* + A^T \xi^* = 0$, we have

$$0 \;=\; (\, c + Qx^*)^T d + \sum_{j=1}^{m} \xi^*_j \, (\, A_{j\bullet} d \,) \;=\; (\, c + Qx^*)^T d.$$

Consequently, it follows that

$$\begin{aligned} q(x^* + \tau d) \;&=\; c^T x^* + \tfrac{1}{2} \, (\, x^* \,)^T Q x^* + \tau \, (\, c + Qx^* \,)^T d + \tfrac{1}{2} \, \tau^2 \, d^T Q d \\ &\leq\; c^T x^* + \tfrac{1}{2} \, (\, x^* \,)^T Q x^* \;=\; \mathrm{QP}_{\min}. \end{aligned}$$

Hence for an appropriate $\tau > 0$ sufficiently small, $x^* + \tau d$ remains an optimal solution to the QP (4.1) and satisfies one more equality $A_{j\bullet} x = b_j$, where $j \notin J_0$, than x^*. Proceeding in this manner, we arrive at either an optimal solution of the QP with a corresponding binary vector belonging to $\mathcal{Z}_2$, or an optimal solution that satisfies all the constraints as binding. In either case, the proposition follows. □

In principle, we could generate more second-order cuts by checking the copositivity of Q on critical cones (this is the original second-order condition for the QP). Instead, we are restricted to the above family $\mathcal{J}$ since checking positive definiteness is much simpler than checking copositivity.

4.3.2 Relaxed LPCC in the sparsification step

As explained in Chapter 3, the sparsification procedure is employed by solving a class of *relaxed LPs with restriction*. Such an LP in the case of QPs is derived from the LPCC problem (4.3) by fixing part of the complementarity conditions at 0 and dropping the rest of them. Whereas the goal of the sparsification step is to obtain a valid satisfiability inequality with as few terms as possible, one must in general balance the work required in this step with the strength of the resulting sparsified inequality. In particular, a judicious choice of the terms which remain in the sparsified inequality is important for the overall efficiency of the algorithm; such a choice remains an open task that deserves further investigation. In Section 4.4.1, we will present a special way of selecting these terms which is employed to the QPs with simple upper and lower bounds by exploring the special structure of its equivalent LPCC formulation.

Suppose the sparser inequality to be tested is given by

$$\sum_{i \in \mathcal{I}} z_i + \sum_{j \in \mathcal{J}} (1 - z_j) \geq 1.$$

We set $z_i = 0$ for all $i \in \mathcal{I}$ and $z_j = 1$ for all $j \in \mathcal{J}$ in (4.12) and restore the complementarity formulation of the resulting restricted IP:

$$\begin{array}{ll} \underset{(x,\xi) \in \Re^{n+m}}{\text{minimize}} & c^T x - b^T \xi \\ \text{subject to} & 0 = c + Qx + A^T \xi \\ & 0 \leq b - Ax \perp \xi \geq 0 \\ & \xi_{\mathcal{J}} = 0 \quad \text{and} \quad (b - Ax)_{\mathcal{I}} = 0, \end{array} \tag{4.13}$$

which remains an LPCC. The complementarity constraints can be relaxed by lifting certain products of variables as follows. More specifically, by defining

$$\zeta_{ik} \equiv x_i \xi_k \quad \text{for all } i, k \text{ such that } a_{ki} \neq 0 \text{ and } k \notin \mathcal{J}, \tag{4.14}$$

we have, for all $k \notin (\mathcal{J} \cup \mathcal{I})$,

$$0 = \xi_k w_k = b_k \xi_k - \sum_{i\,:\,a_{ki} \neq 0} a_{ki}\, \zeta_{ik}.$$

A (very loose) LP relaxation of (4.13) is

$$\begin{array}{ll}
\underset{(x,\xi,y,\zeta)}{\text{minimize}} & c^T x - b^T \xi \\
\text{subject to} & 0 = c + Qx + \sum_{j \notin \mathcal{J}} (\, A_{j\bullet}\,)^T \xi_j \\
& 0 = (\, b - Ax\,)_i, \quad i \in \mathcal{I} \\
& 0 \leq (\, b - Ax\,)_i, \quad i \notin \mathcal{I} \\
& 0 = b_k \xi_k - \sum_{i\,:\,a_{ki} \neq 0} a_{ki}\, \zeta_{ik}, \quad k \notin \mathcal{J} \\
\text{and} & \xi_j \geq 0, \quad j \notin \mathcal{J}.
\end{array}$$

Note that the nonlinear definitions of the variables ζ_{ik} have been dropped in the LP relaxation. Obviously, such a preliminary relaxation cannot be expected to provide tight bounds to the variables in the LP (4.13). Further restriction on these auxiliary variables can be realized by employing some bounding and enveloping techniques developed for handling products of variables. We refer the reader to [73] for such techniques. In what follows, we will specialize the discussion to the problems with bounded variables.

4.4 Simply Constrained QPs

In this section, we restrict our discussion to three special subclasses of indefinite QPs: (a) bounded-variable problems, (b) bounded-variable problems with one additional constraints, and (c) nonnegatively constrained problems (possibly unbounded). We are studying these problems for the following reasons:

• Bounded-variable indefinite QPs have been extensively studied; our goal in this dissertation is to demonstrate that the LPCC approach is a promising new algorithm for resolving these QPs via computational results and comparisons with the recent work [79]. Especially, the LPCC approach can be enhanced by their special structures, leaving room for possible improvement in the future work.

• The class of bounded-variable QPs one additional constraint are chosen to show that the LPCC approach is applicable to general QPs with finite optima. Although, the constraints of these problems are in very special form; yet our discussion sheds light on generalizations which would require further investigation that goes beyond the scope of this thesis.

• The third class of QPs are formulated to provide supporting evidence showing that the LPCC approach is capable of detecting unbounded QPs. This is a task that no practical algorithm is known to be able to accomplish so far.

• Most importantly, our primary goal is to provide evidence supporting the LPCC approach to general indefinite QPs both theoretically and computationally. Although it is not possible to cover this approach with full details in one single work, with the theoretical results in Section 4.2 and the preliminary computational results reported subsequently, we hope to prove the fundamental importance of the LPCC in the treatment of these QPs.

4.4.1 Bounded-variable QPs

Consider the following QP with simple upper and lower bounds:

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}\, x^T Q x + c^T x \\ \text{subject to} & 0 \,\leq\, x \,\leq\, \mathbf{1}_n, \end{array} \tag{4.15}$$

where Q is a symmetric matrix. For $\theta > 0$ sufficiently large, the MIP formulation for this QP is:

$$\begin{array}{ll} \underset{(x,y,z,\lambda)}{\text{minimize}} & c^T x - \mathbf{1}_n^T y \\ \text{subject to} & 0 \leq c + Qx + y \leq \theta\, z \\ & 0 \leq \mathbf{1}_n - x \leq \theta\, \lambda \\ & 0 \leq x \leq \theta\, (\, \mathbf{1}_n - z \,) \\ & 0 \leq y \leq \theta\, (\, \mathbf{1}_n - \lambda \,) \\ \text{and} & z, \lambda \in \{\, 0, 1 \,\}^n. \end{array} \tag{4.16}$$

Since a suitable value for the scalar θ can be easily computed for the above problem, the QP (4.15) can be solved as a mixed integer program. The computational results in [78] show that the a specialized branch-and-cut method proposed in this paper outperforms default MINTO settings. Thus we will use the branch-and-cut method as comparison with the results obtained from our method.

Valid cuts obtained from the pre-processing procedure

In what follows, we discuss the constraints contained in the set $\mathcal{Z}_2$ mentioned in Subsection 4.3.1. These cuts are valid for the MIP (4.16); thus can be added into the SAT problem as permanent cuts. First of all, we have the following cuts:

$$(\, \mathbf{1}_n - z \,) + \lambda \geq \mathbf{1}_n. \quad \text{or equivalently,} \quad \lambda \geq z, \tag{4.17}$$

valid for the MIP problem (4.16), since x cannot be equal 0 and 1 at the same time. Next we focus on the second-order cuts that can be formulated based on the Proposition 16. Noting the difference of the notation used in this proposition from our problem (4.15), the matrix $A = \begin{bmatrix} \mathbf{I}_n \\ -\mathbf{I}_n \end{bmatrix}$; and such index set J in the family $\mathcal{J}$ is taken that $A_{J\bullet}$ consists of all rows of A except for a few pairs of rows of the identity matrix and its negative. As consequences of Proposition 16, we can generate the following sparse cuts in the pre-processing procedure of the algorithm.

• Second-order cuts of order 1. Denote q_{jj} as the jth diagonal entry of Q. If q_{jj} is nonpositive, we have the valid cut $z_j + (1 - \lambda_j) \geq 1$, which, combined with $(1 - z_j) + \lambda_j \geq 1$ from (4.17), leads to $z_j = \lambda_j$. Incidentally, these cuts have been recognized as early as in the work [34] and also used recently in [78, 79]. Nevertheless, the second-order cuts of higher order described below are introduced here for the first time. Note that these are the sparsest second-order cuts that can be derived on the index j. Hence the remaining discussion about the second-order cuts will focus on the positive diagonal entries of matrix Q.

• Second-order cuts of order 2. Suppose q_{ii} and q_{jj} are two positive diagonal entries of Q such that

$$\det \begin{bmatrix} q_{ii} & q_{ij} \\ q_{ji} & q_{jj} \end{bmatrix} \leq 0.$$

Since the above formulated submatrix is not positive definite, the following inequality must be valid:

$$z_i + z_j + (1 - \lambda_i) + (1 - \lambda_j) \geq 1.$$

• Second-order cuts of order 3. Suppose (i, j, k) are 3 distinct indices such that the following three 2×2 matrices:

$$\begin{bmatrix} q_{ii} & q_{ij} \\ q_{ji} & q_{jj} \end{bmatrix}, \quad \begin{bmatrix} q_{ii} & q_{ik} \\ q_{ki} & q_{kk} \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} q_{jj} & q_{jk} \\ q_{kj} & q_{kk} \end{bmatrix}$$

are all positive definite but

$$\det \begin{bmatrix} q_{ii} & q_{ij} & q_{ik} \\ q_{ji} & q_{jj} & q_{jk} \\ q_{ki} & q_{kj} & q_{kk} \end{bmatrix} \leq 0.$$

Similarly we have the following valid cut: $z_i + z_j + z_k + (1 - \lambda_i) + (1 - \lambda_j) + (1 - \lambda_k) \geq 1$.

• Second-order cuts of order ≥ 4. These cuts exist theoretically, but they will not be generated in our algorithm. Firstly, compared with the previous second-order cuts, they contain more terms, thus increasing the complexity of finding a binary vector satisfying the satisfiability system. Secondly, there are too many higher-order principal submatrices, hence it increases the computational difficulty of evaluating these determinants.

As a summary, we obtain the following second-order cuts that are valid to the MIP (4.16) and can be added in permanently:

Valid cuts for (4.16)

(A) $\lambda_j + (1 - z_j) \geq 1$ for all j;

(B) $z_j = \lambda_j$ for all j such that $q_{jj} \leq 0$;

(C) $z_i + z_j + (1 - \lambda_i) + (1 - \lambda_j) \geq 1$ for all $i \neq j$ such that $\min(q_{ii}, q_{jj}) > 0$ and $q_{ij}^2 \geq q_{ii}q_{jj}$;

(D) $z_i + z_j + z_k + (1 - \lambda_i) + (1 - \lambda_j) + (1 - \lambda_k) \geq 1$ for all triples of distinct indices (i, j, k) such that $\min(q_{ii}, q_{jj}, q_{kk}) > 0$, $q_{ij}^2 < q_{ii}q_{jj}$, $q_{ik}^2 < q_{ii}q_{kk}$, $q_{jk}^2 < q_{jj}q_{kk}$, and $q_{ii}q_{jj}q_{kk} + 2q_{ij}q_{jk}q_{ki} - q_{ik}^2 q_{jj} - q_{ij}^2 q_{kk} - q_{jk}^2 q_{ii} \leq 0$.

Point and ray cuts

As illustrated in Chapter 3, based on the solution of the formulated LP $\varphi_0(z)$ ($\varphi(z)$), a ray (point) cut can be derived and added in the satisfiability system. A feasible solution to the modified satisfiability problem provides a new binary vector z to formulate the parameterized $\varphi_0(z)$ ($\varphi(z)$). Such a process is referred as an iteration in our algorithm, which is repeated until a valid certificate of the global resolution is obtained. In the algorithm implemented in Chapter 3 for globally resolving general LPCCs, there is only one point (ray) cut generated within one iteration. However, when implementing the LPCC approach for resolving the bounded-variable QPs, multiple ray cuts can be generated within one iteration. Moreover, due to the special structure of the MIP problem (4.16), we can reduce the size of $\varphi_0(z)$ ($\varphi(z)$) by fixing x at 0 or 1. Introducing dual variables for the linear constraints, we may rewrite the MIP (4.16) as follows:

$$
\begin{array}{llrcll}
\underset{(x,y,z,\lambda)}{\text{minimize}} & & c^T x - \mathbf{1}_n^T y & & & \\
\text{subject to} & & Qx + y & \geq & -c & (\, u^+ \,) \\
& & -Qx - y & \geq & c - \theta\, z & (\, u^- \,) \\
& & -x & \geq & -\mathbf{1}_n & (\, s^+ \,) \\
& & x & \geq & \mathbf{1}_n - \theta\, \lambda, & (\, s^- \,) \\
& & -x & \geq & -\theta\, (\, \mathbf{1}_n - z \,) & (\, v^+ \,) \\
& & -y & \geq & -\theta\, (\, \mathbf{1}_n - \lambda \,) & (\, v^- \,) \\
& & (\, x, y \,) & \geq & 0 & \\
& & (\, \mathbf{1}_n - z \,) + \lambda & \geq & \mathbf{1}_n & \\
\text{and} & & (\, z, \lambda \,) & \in & \{\, 0, 1 \,\}^{2n}. &
\end{array}
$$

For a given binary pair $(z, \lambda) \in \{0,1\}^{2n}$ satisfying $\lambda \geq z$, we define the value function

$$
\begin{array}{rll}
\Re \cup \{\, \infty \,\} \ni \varphi(z,\lambda) \equiv & \underset{(u^\pm, v^\pm, s^\pm)}{\text{maximum}} & c^T(\, u^- - u^+ \,) + \mathbf{1}_n^T(\, s^- - s^+ \,) \\
& \text{subject to} & Q(\, u^+ - u^- \,) - (\, s^+ - s^- \,) - v^+ \,\leq\, c \\
& & u^+ - u^- - v^- \,\leq\, -\mathbf{1}_n \\
& & (\, u^\pm, v^\pm, s^\pm \,) \,\geq\, 0 \\
& \text{and} & z^T u^- + \lambda^T s^- \\
& & \quad +(\, \mathbf{1}_n - z \,)^T v^+ + (\, \mathbf{1}_n - \lambda \,)^T v^- \,\leq\, 0.
\end{array}
$$

Let $\alpha \equiv \text{supp}(z) \subseteq \text{supp}(\lambda) \equiv \gamma$ and $\beta \equiv \gamma \setminus \alpha$. Denote $\bar{\alpha}$ and $\bar{\gamma}$ as the complements of α and γ in $\{1, \cdots, n\}$, respectively. The triplet of index sets $(\alpha, \beta, \bar{\gamma})$ partitions $\{1, \cdots, n\}$, and indicates the three possible states of the variable x: namely, α is the set of indices i for which $x_i = 0$, β is the set of indices i for which $x_i \in (0,1)$, and $\bar{\gamma}$ is the set of indices i for which $x_i = 1$. Due to the complementary slackness conditions between the primal linear constraints and the associated dual variables, any feasible $(u^\pm, v^\pm, s^\pm)$ to $\varphi(z, \lambda)$

must satisfy $u_\alpha^- = 0$, $s_\gamma^- = 0$, $v_{\bar\alpha}^+ = 0$, and $v_{\bar\gamma}^- = 0$. Hence

$$\begin{array}{rll} \varphi(z,\lambda) \equiv & \text{maximum} & -c^T u^+ + c_\beta^T u_\beta^- + c_{\bar\gamma}^T u_{\bar\gamma}^- - \mathbf{1}_n^T s^+ + \mathbf{1}_{|\bar\gamma|}^T s_{\bar\gamma}^- \\ & \text{subject to} & Q_{\alpha\bullet}\, u^+ - Q_{\alpha\beta}\, u_\beta^- - Q_{\alpha\bar\gamma}\, u_{\bar\gamma}^- - s_\alpha^+ - v_\alpha^+ \leq c_\alpha \\ & & Q_{\beta\bullet}\, u^+ - Q_{\beta\beta}\, u_\beta^- - Q_{\beta\bar\gamma}\, u_{\bar\gamma}^- - s_\beta^+ \leq c_\beta \\ & & Q_{\bar\gamma\bullet}\, u^+ - Q_{\bar\gamma\beta}\, u_\beta^- - Q_{\bar\gamma\bar\gamma}\, u_{\bar\gamma}^- - s_{\bar\gamma}^+ + s_{\bar\gamma}^- \leq c_{\bar\gamma} \\ & & u_\alpha^+ - v_\alpha^- \leq -\mathbf{1}_{|\alpha|} \\ & & u_\beta^+ - u_\beta^- - v_\beta^- \leq -\mathbf{1}_{|\beta|} \\ & & u_{\bar\gamma}^+ - u_{\bar\gamma}^- \leq -\mathbf{1}_{|\bar\gamma|} \\ & & (\, u^+, u_\beta^-, u_{\bar\gamma}^-, v_\alpha^+, v_\alpha^-, v_\beta^-, s^+, s_{\bar\gamma}^- \,) \geq 0, \end{array}$$

which can easily be seen to be feasible. Moreover, since the variables v^+ and v^- do not appear in the objective function, we have

$$\begin{array}{rll} \varphi(z,\lambda) \equiv & \text{maximum} & -c^T u^+ + c_\beta^T u_\beta^- + c_{\bar\gamma}^T u_{\bar\gamma}^- - \mathbf{1}_{|\beta|}^T s_\beta^+ - \mathbf{1}_{|\bar\gamma|}^T s_{\bar\gamma}^+ + \mathbf{1}_{|\bar\gamma|}^T s_{\bar\gamma}^- \\ & \text{subject to} & Q_{\beta\bullet}\, u^+ - Q_{\beta\beta}\, u_\beta^- - Q_{\beta\bar\gamma}\, u_{\bar\gamma}^- - s_\beta^+ \leq c_\beta \\ & & Q_{\bar\gamma\bullet}\, u^+ - Q_{\bar\gamma\beta}\, u_\beta^- - Q_{\bar\gamma\bar\gamma}\, u_{\bar\gamma}^- - s_{\bar\gamma}^+ + s_{\bar\gamma}^- \leq c_{\bar\gamma} \\ & & u_{\bar\gamma}^+ - u_{\bar\gamma}^- \leq -\mathbf{1}_{|\bar\gamma|} \\ & & (\, u^+, u_\beta^-, u_{\bar\gamma}^-, s_\beta^+, s_{\bar\gamma}^+, s_{\bar\gamma}^- \,) \geq 0, \end{array}$$

from which we can recover an optimal $(s_\alpha^+, v_\alpha^+, v_\alpha^-, v_\beta^-)$ by letting $s_\alpha^+ = 0$,

$$\begin{aligned} v_\alpha^+ &\equiv \max\left\{ 0, Q_{\alpha\bullet}\, u^+ - Q_{\alpha\beta}\, u_\beta^- - Q_{\alpha\bar\gamma}\, u_{\bar\gamma}^- - c_\alpha \right\} \\ v_\alpha^- &\equiv u_\alpha^+ + \mathbf{1}_{|\alpha|} \\ v_\beta^- &\equiv \max\left\{ 0, u_\beta^+ - u_\beta^- + \mathbf{1}_{|\beta|} \right\}. \end{aligned} \tag{4.18}$$

In turn, by letting

$$\xi_{\bar\gamma} \equiv -\mathbf{1}_{|\bar\gamma|} - u_{\bar\gamma}^+ + u_{\bar\gamma}^- \geq 0, \tag{4.19}$$

and

$$\begin{aligned} s^-_{\bar\gamma} - s^+_{\bar\gamma} \; &\equiv \; c_{\bar\gamma} - Q_{\bar\gamma \bullet}\, u^+ + Q_{\bar\gamma\beta}\, u^-_\beta + Q_{\bar\gamma\bar\gamma}\, u^-_{\bar\gamma} \\ &= \; c_{\bar\gamma} + Q_{\bar\gamma\bar\gamma} \mathbf{1}_{|\bar\gamma|} - Q_{\bar\gamma\alpha}\, u^+_\alpha + Q_{\bar\gamma\beta}\, (\, u^-_\beta - u^+_\beta \,) + Q_{\bar\gamma\bar\gamma}\, \xi_{\bar\gamma} \\ &= \; \bar c_{\bar\gamma} - Q_{\bar\gamma\alpha}\, u^+_\alpha + Q_{\bar\gamma\beta}\, (\, u^-_\beta - u^+_\beta \,) + Q_{\bar\gamma\bar\gamma}\, \xi_{\bar\gamma}. \end{aligned} \tag{4.20}$$

where $\bar c \equiv c + Q_{\bullet\bar\gamma} \mathbf{1}_{|\bar\gamma|}$, we have

$$v^+_\alpha \;\equiv\; \max \left\{ 0, -\bar c_\alpha + Q_{\alpha\alpha}\, u^+_\alpha + Q_{\alpha\beta}\, (\, u^+_\beta - u^-_\beta \,) - Q_{\alpha\bar\gamma}\, \xi_{\bar\gamma} \right\}$$

and

$$\begin{aligned} \varphi(z,\lambda) \;\; &\equiv \;\; 2\, \mathbf{1}^T_{|\bar\gamma|} c_{\bar\gamma} + \mathbf{1}^T_{|\bar\gamma|} Q_{\bar\gamma\bar\gamma} \mathbf{1}_{|\bar\gamma|} + \\ &\qquad \text{maximum} \quad -\bar c^T_\alpha u^+_\alpha + \bar c^T_\beta (\, u^-_\beta - u^+_\beta \,) + \bar c^T_{\bar\gamma} \xi_{\bar\gamma} - \mathbf{1}^T_{|\beta|} s^+_\beta \\ &\qquad \text{subject to} \quad Q_{\beta\alpha}\, u^+_\alpha - Q_{\beta\beta}\, (\, u^-_\beta - u^+_\beta \,) - Q_{\beta\bar\gamma}\, \xi_{\bar\gamma} - s^+_\beta \;\leq\; \bar c_\beta \\ &\qquad \text{and} \quad (\, u^+_\alpha, u^\pm_\beta, \xi_{\bar\gamma}, s^+_\beta \,) \;\geq\; 0 \\ &= \;\; 2\, \mathbf{1}^T_{|\bar\gamma|} c_{\bar\gamma} + \mathbf{1}^T_{|\bar\gamma|} Q_{\bar\gamma\bar\gamma} \mathbf{1}_{|\bar\gamma|} + \\ &\qquad \text{minimum} \quad \bar c^T_\beta \widehat{x}_\beta \\ &\qquad \text{subject to} \quad \bar c_\alpha + Q_{\alpha\beta}\, \widehat{x}_\beta \;\geq\; 0, \qquad (\, u^+_\alpha \,) \\ &\qquad\qquad \bar c_\beta + Q_{\beta\beta}\, \widehat{x}_\beta \;=\; 0, \qquad (\, \xi_\beta \,) \\ &\qquad\qquad \bar c_{\bar\gamma} + Q_{\bar\gamma\beta}\, \widehat{x}_\beta \;\leq\; 0, \qquad (\, \xi_{\bar\gamma} \,) \\ &\qquad \text{and} \quad \mathbf{1}_{|\beta|} \;\geq\; \widehat{x}_\beta \;\geq\; 0. \end{aligned}$$

In reduced variables and constraints, the linear program

$$\begin{aligned} &\text{maximize} \quad -\bar c^T_\alpha u^+_\alpha + \bar c^T_\beta (\, u^-_\beta - u^+_\beta \,) + \bar c^T_{\bar\gamma} \xi_{\bar\gamma} - \mathbf{1}^T_{|\beta|} s^+_\beta \\ &\text{subject to} \quad Q_{\beta\alpha}\, u^+_\alpha - Q_{\beta\beta}\, (\, u^-_\beta - u^+_\beta \,) - Q_{\beta\bar\gamma}\, \xi_{\bar\gamma} - s^+_\beta \;\leq\; \bar c_\beta \\ &\text{and} \quad (\, u^+_\alpha, u^\pm_\beta, \xi_{\bar\gamma}, s^+_\beta \,) \;\geq\; 0, \end{aligned} \tag{4.21}$$

or its dual, can be used to generate the valid point cuts. Let $(\widehat{u}_\alpha^{p,+}, \widehat{u}_\beta^{p,\pm}, \widehat{\xi}_{\bar{\gamma}}^{p}, \widehat{s}_\beta^{p,+})$ be an optimal extreme point solution of (4.21). From (4.18) and (4.20), we define

$$\begin{aligned}
\widehat{s}_{\bar{\gamma}}^{p,-} &\equiv \max\left\{ 0,\, \bar{c}_{\bar{\gamma}} - Q_{\bar{\gamma}\alpha}\, \widehat{u}_\alpha^{p,+} + Q_{\bar{\gamma}\beta}\,(\, \widehat{u}_\beta^{p,-} - \widehat{u}_\beta^{p,+}\,) + Q_{\bar{\gamma}\bar{\gamma}}\, \widehat{\xi}_{\bar{\gamma}}^{p} \right\} \\
\widehat{v}_\alpha^{p,+} &\equiv \max\left\{ 0, -\bar{c}_\alpha + Q_{\alpha\alpha}\, \widehat{u}_\alpha^{p,+} - Q_{\alpha\beta}\,(\, \widehat{u}_\beta^{p,-} - \widehat{u}_\beta^{p,+}\,) - Q_{\alpha\bar{\gamma}}\, \widehat{\xi}_{\bar{\gamma}}^{p} \right\} \\
\widehat{v}_\beta^{p,-} &\equiv \max\left\{ 0, \widehat{u}_\beta^{p,+} - \widehat{u}_\beta^{p,-} + \mathbf{1}_{|\beta|} \right\}.
\end{aligned}$$

Moreover, based on (4.18) and (4.19), we have:

$$\begin{aligned}
\widehat{u}_{\bar{\gamma}}^{p,-} &= \widehat{\xi}_{\bar{\gamma}}^{p} + \widehat{u}_{\bar{\gamma}}^{p,+} + \mathbf{1}_{\bar{\gamma}} &> 0 \\
\widehat{v}_\alpha^{p,-} &= \widehat{u}_\alpha^{p,+} + \mathbf{1}_\alpha &> 0.
\end{aligned}$$

Thus, the obtained point cut is:

$$\begin{aligned}
&\sum_{i \in \bar{\gamma}} z_i + \sum_{i \in \beta : \widehat{u}_i^{p,-} > 0} z_i + \sum_{i \in \bar{\gamma} : \widehat{s}_i^{p,-} > 0} \lambda_i + \\
&\qquad \sum_{i \in \alpha : \widehat{v}_i^{p,+} > 0} (\, 1 - z_i\,) + \sum_{i \in \beta : \widehat{v}_i^{p,-} > 0} (\, 1 - \lambda_i\,) + \sum_{i \in \alpha} (\, 1 - \lambda_i\,) \,\geq\, 1.
\end{aligned}$$

Valid ray cuts can be obtained by identifying a feasible ray of (4.21) on which the objective is unbounded above. In order to generate multiple ray cuts for one given binary vector (z, λ), we solve a modified LP of (4.21) by replacing the right hand side of the constraints with 0 and letting the objective be equal to a given positive scalar σ. The new obtained LP is thus:

$$\begin{array}{ll}
\text{maximize} & 0 \\
\text{subject to} & Q_{\beta\alpha}\, u_\alpha^+ - Q_{\beta\beta}\,(\, u_\beta^- - u_\beta^+\,) - Q_{\beta\bar{\gamma}}\, \xi_{\bar{\gamma}} - s_\beta^+ \,\leq\, 0 \\
& -\bar{c}_\alpha^T u_\alpha^+ + \bar{c}_\beta^T(\, u_\beta^- - u_\beta^+\,) + \bar{c}_{\bar{\gamma}}^T \xi_{\bar{\gamma}} - \mathbf{1}_{|\beta|}^T s_\beta^+ \,=\, \delta \\
\text{and} & (\, u_\alpha^+, u_\beta^\pm, \xi_{\bar{\gamma}}, s_\beta^+\,) \,\geq\, 0.
\end{array} \tag{4.22}$$

Note that the above LP (4.22) is either infeasible, if (4.21) attains finite optima; or feasible with a finite optimal solution if (4.21) is unbounded. In the latter case, any extreme point of (4.22) will constitute a feasible ray of the LP (4.21) on which the objective is unbounded. Thus we can use any function as the objective of (4.22). Suppose by solving (4.22), the solution $(\widehat{u}_{\alpha}^{r,+}, \widehat{u}_{\beta}^{r,\pm}, \widehat{\xi}_{\bar{\gamma}}^{r}, \widehat{s}_{\beta}^{r,+})$ is obtained as an extreme ray of (4.21). Define

$$\begin{aligned}
\widehat{s}_{\bar{\gamma}}^{r,-} &\equiv \max\left\{ 0,\, -Q_{\bar{\gamma}\alpha}\, \widehat{u}_{\alpha}^{r,+} + Q_{\bar{\gamma}\beta}\,(\,\widehat{u}_{\beta}^{r,-} - \widehat{u}_{\beta}^{r,+}\,) + Q_{\bar{\gamma}\bar{\gamma}}\, \widehat{\xi}_{\bar{\gamma}}^{r} \right\} \\
\widehat{v}_{\alpha}^{r,+} &\equiv \max\left\{ 0, Q_{\alpha\alpha}\, \widehat{u}_{\alpha}^{r,+} - Q_{\alpha\beta}\,(\,\widehat{u}_{\beta}^{r,-} - \widehat{u}_{\beta}^{r,+}\,) - Q_{\alpha\bar{\gamma}}\, \widehat{\xi}_{\bar{\gamma}}^{r} \right\} \\
\widehat{u}_{\bar{\gamma}}^{r,-} &\equiv \widehat{\xi}_{\bar{\gamma}}^{r} \\
\widehat{v}_{\alpha}^{r,-} &\equiv \widehat{u}_{\alpha}^{r,+} \\
\widehat{v}_{\beta}^{r,-} &\equiv \widehat{u}_{\beta}^{r,+}.
\end{aligned} \tag{4.23}$$

The ray cut is then:

$$\sum_{i\in\bar{\alpha}:\widehat{u}_i^{r,-}>0} z_i + \sum_{i\in\bar{\gamma}:\widehat{s}_i^{r,-}>0} \lambda_i + \sum_{i\in\alpha:\widehat{v}_i^{r,+}>0} (\,1 - z_i\,) + \sum_{i\in\gamma:\widehat{v}_i^{r,-}>0} (\,1 - \lambda_i\,) \geq 1. \tag{4.24}$$

A very interesting case is when the value of $\widehat{s}_i^{r,-}$ $(i \in \bar{\gamma})$ is positive but strictly less than δ, the corresponding term λ_i in the formulated ray cut (4.24) can be deleted, and the resulting sparser constraint still remains as a valid ray cut for the MIP (4.16). This can be proved by conducting a simple pivoting step in the problem (4.22). Similarly, we can delete the term $(1 - z_i)$ from (4.24) as long as the value of $\widehat{v}_i^{r,+}$ $(i \in \alpha)$ is strictly less than δ. Based on this observation, we can sparsify the obtained ray cut (4.24) by deleting the terms of λ_i and $(1 - z_i)$ which have the corresponding variables $\widehat{s}^{r,-}$ and $\widehat{v}^{r,+}$ summing to the value that is strictly less than δ.

Moreover, multiple valid ray cuts can be generated by fixing at 0 one of the variables from the set of $\{u_{\bar{\alpha}}^{r,-},\, s_{\bar{\gamma}}^{r,-},\, v_{\alpha}^{r,+},\, v_{\gamma}^{r,-}\}$ which are strictly positive in the obtained solution. Note that for the variables that do not appear in the problem (4.22), we can instead add in one constraint; i.e., fixing $s_i^{r,-}$ at 0 is equivalent to the addition of the following constraint into the problem (4.22):

$$-Q_{i\alpha}\, \widehat{u}_{\alpha}^{r,+} + Q_{i\beta}\,(\,\widehat{u}_{\beta}^{r,-} - \widehat{u}_{\beta}^{r,+}\,) + Q_{i\bar{\gamma}}\, \widehat{\xi}_{\bar{\gamma}}^{r} \leq 0.$$

In the empirical experiments, we found that, by choosing one of the variables $\{u_{\bar{\alpha}}^{r,-},\ v_{\gamma}^{r,-}\}$ to fix, the obtained ray cuts have more varieties than the other options. Also it is more desirable if the next obtained ray cut is most different than the cuts that already exist in the satisfiability system. For this purpose, we can fix the variable among $\{u_{\bar{\alpha}}^{r,-},\ v_{\gamma}^{r,-}\}$, which has the corresponding term z_i or $(1-\lambda_i)$ in the cut (4.24) appearing most frequently in the satisfiability problem. The detail of the procedure is summarized as follows.

Step 1. If problem (4.22) is infeasible, break.

Step 2. Suppose, based on the optimal solution of (4.22), a valid ray cut is formulated as (4.24). Sort out the variables $\{\widehat{s}_{\bar{\gamma}}^{r,-}\}$ and $\{\widehat{v}_{\alpha}^{r,+}\}$ with respect to their values in the optimal solution. Take the variables $\{\widehat{s}_{\bar{\gamma}}^{r,-}\}$ and $\{\widehat{v}_{\alpha}^{r,+}\}$ that have the least values and the sum strictly less than δ (a tolerance of 10^{-6} can be used here) and delete the corresponding terms of λ_i or $(1-z_i)$ from (4.24). The obtained sparser cut is a valid ray cut and will be used for the sparsification step.

Step 3. Among the terms z_i and $(1-\lambda_i)$ appearing in (4.24), choose the term that appears most frequently in the satisfiability problem. Fix the corresponding variable $\widehat{u}_i^{r,-}$ or $\widehat{v}_i^{r,-}$ at 0. Go to *step 1.*

Sparsification of the satisfiability constraint

As presented in Chapter 3, sparsification is a procedure that requires solving sub-linear programs. Thus one needs to balance the extra computational work and the benefits of the process. For this purpose, firstly, we only apply the sparsification step to the valid ray cuts, for instance (4.24), which are obtained by solving the problem (4.22). Secondly, a specialized procedure is implemented to formulate the sub-inequality, which is a sparsification of the ray cut. The validity of the sub-inequality is tested by solving a corresponding relaxed LP with restriction. From the empirical experiments, we found that the sparsification step has a better chance to succeed by leaving the terms z_i and $(1-\lambda_i)$ in the sub-inequality, and retaining the terms λ_i and $(1-z_i)$ which have the corresponding $s_i^{r,-}$ and $v_i^{r,+}$ with larger values among the variables $\{s_{\bar{\gamma}}^{r,-},\ v_{\alpha}^{r,+}\}$. Based on this observation, we summarize the sparsification procedure as follows.

Step 1. Retain the terms z_i and $(1-\lambda_i)$ in the sub-inequality.

Step 2. Sort out the variables $\{\widehat{s}^{r,-}_{\bar{\gamma}}\}$ and $\{\widehat{v}^{r,+}_{\alpha}\}$ with respect to their values in the optimal solution of (4.22). Sum up the values of these variables and obtain a value, say v. Retain the terms $(1-z_i)$ and λ_i in the sub-inequality, such that the corresponding variables $\widehat{s}^{r,-}_i$ and $\widehat{v}^{r,+}_i$ add up to more than $0.5v$ and that with one less term the sum would be less than $0.5v$.

Step 3. Based on the terms that appear in the sub-inequality, formulate the relaxed LP with restriction. The solution of this problem has two different states: infeasible or bounded with a finite optimal solution. For the first state, by standard conversion, we define the objective value $\mathrm{LP}_{\mathrm{rlx}}$ to be ∞. There are two cases associated with $\mathrm{QP}_{\mathrm{ub}}$, which denotes the current upper bound of the bounded-variable problem (4.15):

- $\mathrm{LP}_{\mathrm{rlx}} < \mathrm{QP}_{\mathrm{ub}}$: Place this constraint into the waiting pool for future verification and add the original ray cut into the satisfiability problem. Starting from the optimal solution of the relaxed LP, do a steepest-descent local search until a stationary point is obtained. If a better local solution of the bounded-variable problem (4.15) is found, update $\mathrm{QP}_{\mathrm{ub}}$.
- $\mathrm{QP}_{\mathrm{ub}} \leq \mathrm{LP}_{\mathrm{rlx}}$: The sparsification is successful and we can add the sub-inequality as a valid cut into the satisfiability problem.

A simple numerical example is given as follows to illustrate how to construct the sub-inequality. Suppose the ray cut is:

$$z_1 + \lambda_2 + \lambda_4 + (1-z_3) + (1-z_6) + (1-\lambda_8) \geq 1,$$

with the corresponding variables: $\widehat{s}^{r,-}_2 = 25.0$, $\widehat{s}^{r,-}_4 = 40.0$, $\widehat{v}^{r,+}_3 = 20.0$ and $\widehat{v}^{r,+}_6 = 50.0$. The terms z_1 and $(1-\lambda_8)$ will remain in the sub-inequality. After sorting out the variables $\widehat{s}^{r,-}_2$, $\widehat{s}^{r,-}_4$, $\widehat{v}^{r,+}_3$ and $\widehat{v}^{r,+}_6$, we can decide that λ_4 and $(1-z_6)$ will stay in the sub-inequality.

Thus, the obtained sparser cut to be tested is formulated as:

$$z_1 \,+\, \lambda_4 \,+\, (1 - z_6) \,+\, (1 - \lambda_8) \,\geq\, 1.$$

In what follows, we will explain how to formulate the relaxed LP based on the sub-inequality to be tested. Suppose that we want to test the validity of the satisfiability inequality:

$$\sum_{i \in \mathcal{I}_1} z_i + \sum_{i \in \mathcal{I}_2} (\, 1 - z_i \,) + \sum_{i \in \mathcal{J}_1} \lambda_i + \sum_{i \in \mathcal{J}_2} (\, 1 - \lambda_i \,) \,\geq\, 1. \tag{4.25}$$

Since $\lambda \geq z$, it suffices to consider the case where $\mathcal{I}_2 \cap \mathcal{J}_1 = \emptyset$. To accomplish this test, we assume the contrary, i.e., assume

$$\sum_{i \in \mathcal{I}_1} z_i + \sum_{i \in \mathcal{I}_2} (\, 1 - z_i \,) + \sum_{i \in \mathcal{J}_1} \lambda_i + \sum_{i \in \mathcal{J}_2} (\, 1 - \lambda_i \,) \,\leq\, 0, \tag{4.26}$$

and consider the LPCC resulting from setting the corresponding variables in the respective index sets equal to zero, i.e., $z_i = 0$ for all $i \in \mathcal{I}_1$, $z_i = 1$ for all $i \in \mathcal{I}_2$; $\lambda_i = 0$ for all $i \in \mathcal{J}_1$, and $\lambda_i = 1$ for all $i \in \mathcal{J}_2$:

$$\begin{array}{ll}
\underset{(x,y)}{\text{minimize}} & c^T x - \mathbf{1}_n^T y \\
\text{subject to} & 0 \,\leq\, c + Qx + y \,\perp\, x \,\geq\, 0 \\
 & 0 \,\leq\, \mathbf{1}_n - x \,\perp\, y \,\geq 0 \\
 & (\, c + Qx + y \,)_i \,=\, 0, \quad \forall\, i \,\in\, \mathcal{I}_1 \\
 & 1 - x_i \,=\, 0, \qquad\qquad \forall\, i \,\in\, \mathcal{J}_1 \\
 & x_i \,=\, 0, \qquad\qquad\quad \forall\, i \,\in\, \mathcal{I}_2 \\
 & y_i \,=\, 0, \qquad\qquad\quad \forall\, i \,\in\, \mathcal{J}_2
\end{array} \tag{4.27}$$

With some of the x-variables fixed, the complementarity condition could be used to fix further variables, using the following implications:

$$[\, x_i \,=\, 1 \,\Rightarrow\, (\, c + Qx + y \,)_i \,=\, 0 \,] \quad \text{and} \quad [\, x_i \,=\, 0 \,\Rightarrow\, y_i \,=\, 0 \,]. \tag{4.28}$$

Thus (4.27) is equivalent to:

$$\begin{array}{lll}
\underset{(x,y)}{\text{minimize}} & c^T x - \mathbf{1}_n^T y & \\
\text{subject to} & 0 \leq c + Qx + y \perp x \geq 0 & \\
& 0 \leq \mathbf{1}_n - x \perp y \geq 0 & \\
& (c + Qx + y)_i = 0, & \forall\, i \in \mathcal{I}_1 \\
& 1 - x_i = 0 = (c + Qx + y)_i, & \forall\, i \in \mathcal{J}_1 \\
& x_i = 0 = y_i, & \forall\, i \in \mathcal{I}_2 \\
& y_i = 0, & \forall\, i \in \mathcal{J}_2
\end{array} \tag{4.29}$$

Further implications and fixings of variables can be derived by two approaches. The first approach is based on the valid cuts that already exist in the satisfiablity system. To illustrate, suppose that the inequality $z_1 + (1 - z_2) + \lambda_3 \geq 1$ is known to be valid and we are testing the inequality $z_1 + (1 - z_2) + (1 - \lambda_4) \geq 1$. Setting $z_1 = 1 - z_2 = 1 - \lambda_4 = 0$ yields, by the former valid inequality, $\lambda_3 = 0$, meaning that we can set $x_3 = 1$ additionally. This procedure has been observed in the numerical experiments to improve the computational time by nearly 50% over the algorithm without this procedure, particularly when there already exist certain amount of sparse cuts in the satisfiability problem. Note that the first set of implications (4.28) can be treated as a special case here, since we always have $(1 - z_i) + \lambda_i \geq 1$ $i = 1 \ldots n$ as valid cuts.

The second approach is based on the special structure of the formulated LP (4.29) by noting:

$$\begin{aligned}
c_i + \sum_{j=1}^{n} q_{ij}\, x_j &= c_i + \sum_{j \in \mathcal{J}_1} q_{ij} + \sum_{\substack{j \notin (\mathcal{I}_2 \cup \mathcal{J}_1) \\ q_{ij} \neq 0}} q_{ij}\, x_j \\
&\geq c_i + \sum_{j \in \mathcal{J}_1} q_{ij} + \sum_{\substack{j \notin (\mathcal{I}_2 \cup \mathcal{J}_1) \\ q_{ij} < 0}} q_{ij} \equiv \sigma_i^+.
\end{aligned}$$

Similarly,

$$c_i + \sum_{j=1}^{n} q_{ij}\, x_j \leq \sum_{j \in \mathcal{J}_1} q_{ij} + \sum_{\substack{j \notin (\mathcal{I}_2 \cup \mathcal{J}_1) \\ q_{ij} > 0}} q_{ij} \equiv \sigma_i^-.$$

The implications below must be valid for the problem (4.29):

$$\left[\,\sigma_i^+ \,=\, 0 \;\Rightarrow\; y_i \,=\, 0\,\right], \qquad\qquad \left[\,\sigma_i^+ \,>\, 0 \;\Rightarrow\; x_i \,=\, 0 \,=\, y_i\,\right]$$
$$\left[\,\sigma_i^- \,=\, 0 \;\Rightarrow\; (\,c + Qx + y\,)_i \,=\, 0\,\right], \quad \left[\,\sigma_i^- \,<\, 0 \;\Rightarrow\; x_i \,=\, 1\,\right]$$

We next consider a relaxation of the complementarity constraint that are not fixed yet by the former implications. For an index i, suppose neither x_i nor $(c + Qx + y)_i$ can be fixed:

$$\begin{aligned} 0 &= x_i\,(\,c + Qx + y\,)_i \\ &= \left(c_i + \sum_{j \in \mathcal{J}_1} q_{ij} \right) x_i + \sum_{\substack{q_{ij} \neq 0 \\ j:x_j \text{ not yet fixed}}} q_{ij}\, w_{ij} + y_i, \end{aligned}$$

where $w_{ij} \equiv x_i x_j$ for all i and j such that x_i and x_j are not yet fixed and such that $q_{ij} \neq 0$. The nonlinear equation $w_{ij} \equiv x_i x_j$ can be relaxed by replacing it with the following linear constraints:

$$\max(\,0, x_i + x_j - 1\,) \;\leq\; w_{ij} \;\leq\; \min(\,x_i, x_j\,).$$

Additional restrictions on the variables w_{ij} may be imposed to tighten the feasible region of the relaxed LP. More specifically, if both w_{ii} (if $q_{ii} \neq 0$) and w_{jj} (if $q_{jj} \neq 0$) are well defined, then we have $w_{ii} + w_{jj} \geq 2w_{ij}$ and $(x_i + x_j)^2 \leq w_{ii} + 2w_{ij} + w_{jj}$ as two valid constraints. While the latter is a nonlinear constraint, it is convex and of the second-order cone (SOC) type, which can be effectively handled by state-of-the-art SOC computer softwares. One last constraint that can be added is based on the implication:

$$q_{ii} \,<\, 0 \;\Rightarrow\; [\,x_i \,=\, 0 \text{ or } 1\,] \;\Rightarrow\; w_{ii} \,=\, x_i.$$

Collecting all the above implied variable fixings and linear constraints on the auxiliar variables w_{ij}, we arrive at the following LP relaxation of (4.29):

$$
\begin{array}{ll}
\underset{(x,y,w)}{\text{minimize}} & c^T x - \mathbf{1}_n^T y \\
\text{subject to} & 0 \leq c + Qx + y, \quad x \geq 0 \\
& 0 \leq \mathbf{1}_n - x, \quad y \geq 0 \\
& 0 = \left(c_i + \displaystyle\sum_{j \in \mathcal{J}_1} q_{ij} \right) x_i + \displaystyle\sum_{\substack{q_{ij} \neq 0 \\ j : x_j \text{ not fixed}}} q_{ij}\, w_{ij} + y_i, \quad \forall\, i \text{ with } x_i \text{ not fixed} \\
\text{plus} & \text{fixed complementarities; cf. (4.27)} \\
\text{and} & \text{all implied variable fixings and linear constraints on } w_{ij} \text{ as described above.}
\end{array}
\tag{4.30}
$$

If the optimal objective value of the LP (4.30) exceeds a valid upper bound of $\text{QP}_{\min}$, then the satisfiability constraint (4.25) is valid and can be added to the overall satisfiability system to determine the next LP piece to continue the search.

Local search

When solving the LP (4.30), it is possible that the obtained optimal solution $(\widetilde{x}, \widetilde{y})$ fails to satisfy the complementarity conditions, since some of these conditions have been relaxed. Thus, $(\widetilde{x}, \widetilde{y})$ is not a KKT pair of the QP (4.15). When this happens, we can apply a local search method, such as a simple gradient projection iteration initiated at $\widetilde{x}$, to recover a KKT pair. This local search is the *feasibility recovery step* described in Chapter 3 for the general LPCC, which in this case can be implemented by a standard local method for QPs. A local search is also employed to obtain an initial value of QP_{ub} at the beginning of the algorithm.

4.4.2 Bounded-variable QPs with 1 constraint

Consider the following bounded-variable QP with one additional inequality constraint:

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}\, x^T Q x + c^T x \\ \text{subject to} & 0 \,\leq\, x \,\leq\, \mathbf{1}_n \\ \text{and} & \mathbf{1}_n^T x \,\leq\, f \end{array} \tag{4.31}$$

where Q is symmetric and f is a positive scalar. The MIP formulation for this QP is: for $\theta > 0$ sufficiently large,

$$\begin{array}{ll} \underset{(x,y,z,\lambda)}{\text{minimize}} & c^T x - \mathbf{1}_n^T y \\ \text{subject to} & 0 \,\leq\, c + Qx + y + \mathbf{1}_n\, \eta \,\leq\, \theta\, z \\ & 0 \,\leq\, \mathbf{1}_n - x \,\leq\, \theta\, \lambda \\ & 0 \,\leq\, f - \mathbf{1}_n^T x \,\leq\, \theta\, \lambda_{n+1} \\ & 0 \,\leq\, x \,\leq\, \theta\, (\, \mathbf{1}_n - z\,) \\ & 0 \,\leq\, y \,\leq\, \theta\, (\, \mathbf{1}_n - \lambda\,) \\ & 0 \,\leq\, \eta \,\leq\, \theta\, (\, 1 - \lambda_{n+1}\,) \\ \text{and} & z, \lambda \,\in\, \{\, 0, 1\, \}^n, \quad \lambda_{n+1} \,\in\, \{\, 0, 1\, \}. \end{array} \tag{4.32}$$

We can establish valid cuts for (4.32) as a pre-processor similarly to the bounded-variable problem. The difference lies in the notation of matrix of A, which, compared to the bounded-variable problem (4.15), has one extra row; namely, $A = \begin{bmatrix} \mathbf{I}_n \\ -\mathbf{I}_n \\ -\mathbf{1}_n^T \end{bmatrix}$. Thus the extra term $(1 - \lambda_{n+1})$ is needed in each of the cases described in the Section 4.4.1. In principle, cuts without this extra term can be proved to be valid under more restrictive conditions; for instance, if $\min(q_{ii}, q_{jj}) > 0$ and $q_{ii} + q_{jj} \leq 2q_{ij}$, where the latter condition is equivalent to saying that the 2×2 matrix

$$\begin{bmatrix} q_{ii} & q_{ij} \\ q_{ji} & q_{jj} \end{bmatrix}$$

is not positive definite on the null space $x_i + x_j = 0$, then the constraint $z_i + z_j + (1 - \lambda_i) + (1 - \lambda_j) \geq 1$ is valid. Similarly, suppose (i, j, k) are 3 distinct indices such that the following three 2×2 matrices:

$$\begin{bmatrix} q_{ii} & q_{ij} \\ q_{ji} & q_{jj} \end{bmatrix}, \quad \begin{bmatrix} q_{ii} & q_{ik} \\ q_{ki} & q_{kk} \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} q_{jj} & q_{jk} \\ q_{kj} & q_{kk} \end{bmatrix}$$

are all positive definite but

$$\begin{bmatrix} q_{ij} & q_{ij} & q_{ik} \\ q_{ji} & q_{jj} & q_{jk} \\ q_{ki} & q_{kj} & q_{kk} \end{bmatrix}$$

is not positive definite on the subspace: $x_i + x_j + x_k = 0$, or equivalently, if the matrix

$$\begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} q_{ii} & q_{ij} & q_{ik} \\ q_{ji} & q_{jj} & q_{jk} \\ q_{ki} & q_{kj} & q_{kk} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} q_{ii} - 2q_{ij} + q_{jj} & q_{ij} - q_{ik} - q_{jj} + q_{jk} \\ q_{ji} - q_{ki} - q_{jj} + q_{kj} & q_{jj} - 2q_{jk} + q_{kk} \end{bmatrix}$$

is not positive definite, then the constraint $z_i + z_j + z_k + (1 - \lambda_i) + (1 - \lambda_j) + (1 - \lambda_k) \geq 1$ is valid. The generation of valid cuts for the MIP problem (4.32) can be summarized as follows.

Valid cuts for (4.32)

(A) $\lambda_j + (1 - z_j) \geq 1$ for all j;

(B) $z_j + (1 - \lambda_j) + (1 - \lambda_{n+1}) \geq 1$ for all j such that $q_{jj} \leq 0$;

(C) $z_i + z_j + (1 - \lambda_i) + (1 - \lambda_j) + (1 - \lambda_{n+1}) \geq 1$ for all $i \neq j$ such that $\min(q_{ii}, q_{jj}) > 0$ and $q_{ij}^2 \geq q_{ii}q_{jj}$;

(D) $z_i + z_j + z_k + (1 - \lambda_i) + (1 - \lambda_j) + (1 - \lambda_k) + (1 - \lambda_{n+1}) \geq 1$ for all triples of distinct indices (i, j, k) such that $\min(q_{ii}, q_{jj}, q_{kk}) > 0$, $q_{ij}^2 < q_{ii}q_{jj}$, $q_{ik}^2 < q_{ii}q_{kk}$, $q_{jk}^2 < q_{jj}q_{kk}$, and $q_{ii}q_{jj}q_{kk} + 2q_{ij}q_{jk}q_{ki} - q_{ik}^2 q_{jj} - q_{ij}^2 q_{kk} - q_{jk}^2 q_{ii} \leq 0$.

(E) Additional cuts corresponding to other choices of the index set J in the family $\mathcal{J}$ may be added, including those similar to (C) and (D) but without the $(1 - \lambda_{n+1})$ term.

The sparsification procedure for this class of problems is similar to the procedure implemented for solving the bounded-variable problems. The only difference is that the extra terms $(1 - \lambda_{n+1})$ and z_{n+1}, if any of them appreas in the ray cut to be sparsified, will be kept in the sub-inequality. The details are not repeated here.

4.4.3 Nonnegatively constrained, copositive QPs

Consider the following nonnegatively constrained QP:

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}\, x^T Q x + c^T x \\ \text{subject to} & x \geq 0, \end{array} \tag{4.33}$$

where Q is symmetric and copositive. This problem either attains a finite optimal solution or is unbounded below. By Corollary 14, the resolution of this dichotomy can be determined by solving the LPCC:

$$
\begin{array}{lll}
\underset{(x,d,t)\in\Re^{2n+1}}{\text{minimize}} & -t & \\
\text{subject to} & \mathbf{1}_n^T d \,\geq\, 1 & \\
& 0 \,\leq\, c + Qx + t\,\mathbf{1}_n \,\perp\, x \,\geq 0 & \\
& 0 \,\leq\, Qd \,\perp\, d \,\geq 0 & \\
\text{and} & c + Qx + t\,\mathbf{1}_n \,\perp\, d. &
\end{array} \tag{4.34}
$$

whose MIP formulation is:

$$
\begin{array}{ll}
\underset{(x,d,z,\lambda,t)\in\Re^{4n+1}}{\text{minimize}} & -t \\
\text{subject to} & \mathbf{1}_n^T d \,\geq\, 1 \\
& 0 \,\leq\, c + Qx + t\,\mathbf{1}_n \,\leq\, \theta\, z \\
& 0 \,\leq\, x \,\leq\, \theta\,(\,\mathbf{1}_n - z\,) \\
& 0 \,\leq\, Qd \,\leq\, \theta\,\lambda \\
& 0 \,\leq\, d \,\leq\, \theta\,(\,\mathbf{1}_n - \lambda\,) \\
& d \,\leq\, \theta\,(\,\mathbf{1}_n - z\,) \\
\text{and} & (\,z,\lambda\,) \,\in\, \{\,0,1\,\}^{2n}.
\end{array} \tag{4.35}
$$

Note that if $z_i = 1$, then $d_i = 0$; hence we may take $\lambda_i = 1$. Thus, the constraint $\lambda \geq z$ is always a valid cut for (4.35), and can be added in the satisfiability system before the main algorithm. While it may be possible to derive other cuts for this MIP, we have not investigated this problem as thoroughly as the other two classes of QPs. In the numerical results, we solved the LPCC (4.34) using the general algorithm sketched at the beginning of Section 4.3.

4.5 Computational Results

In the Section 4.3, we have presented the algorithms specialized to solving three different classes of QPs. These algorithms are coded in a C-environment and implemented with two interfaces: CPLEX 10.0 for solving the LPs and zChaff 3.12 for solving the satisfiability problems. With the Chaff algorithm implemented, zChaff is designed for solving the boolean satisfiability problem and free for non-commercial use. It can be downloaded from the website: http://www.princeton.edu/ chaff/zchaff.html. The experiments were run on a Dell desktop computer with a Core Duo CPU, 2.33 GHz processor, and 1.95 GB of RAM. The data for the bounded-variable QPs are the same as those in [79]; in particular, the entries of Q and c are randomly generated integers between -50 and 50. The experiments in this reference were run on a SUN Ultra-80 with 2x450-MHz UltraSPARC-II processors and 1-GB Memory. The same data was used for the bound-variable QPs with one additional inequality constraint, where the right-hand constant f of this constraint, as referenced in (4.31), is set to be $n/2$. There are two sets of problems solved for the class of nonnegatively constrained, copositive QPs. The data for the first set of these problems are generated as follows. The 2×2 leading principal submatrix of the matrix Q in each problem is $\begin{bmatrix} 25 & -25 \\ -25 & 25 \end{bmatrix}$. The remaining entries are nonnegative integers between 0 and 50. Thus the matrix Q is copositive on the nonnegative orthant, and not necessarily positive semidefinite. The first two entries of the vector c are -2 and 1; the rest of the entries of c are randomly generated integers between -20 and 20. Therefore, this group of QPs have the objetive unbounded on the feasible ray $(1,\, 1,\, 0 \cdots 0)$. Note that stationary solutions may or may not exist for this set of problems. Interested in the case when the nonnegatively constrained, copositive QPs are guaranteed to have stationary solution but remain unbounded, we modified the data of the first set of such QPs as follows. The matrix Q has

$$Q_3 \equiv \begin{bmatrix} 25 & -25 & 50 \\ -25 & 25 & -25 \\ 50 & -25 & 25 \end{bmatrix}$$

as its leading 3×3 principal submatrix and the remaining entries of Q are generated in the same way as before; the vector $c = -Qx^0$, where x^0 is the vector with the first 3 components equal to 1 and the rests equal zero. As a result, the first 3 components of c are equal to -50, 25, and 50. The modified QP remains unbounded on the ray $(1,\, 1,\, 0 \cdots 0)$

and has x^0 as a stationary solution satisfing the KKT condition: $0 \leq x \perp Qx + c \geq 0$. The matrix Q_3 is copositive because

$$\left(\begin{array}{ccc} d_1 & d_2 & d_3 \end{array} \right) Q_3 \left(\begin{array}{c} d_1 \\ d_2 \\ d_3 \end{array} \right) = 25\,(\,d_1 - d_2 + d_3\,)^2 + 50\,d_1 d_3 \,\geq\, 0$$

for all $(d_1, d_3) \geq 0$.

Tables 4.1–4.4 report the computational results for the bounded-variable QPs with 30, 40, 50, and 60 variables, respectively. The results contained in each table are reported in the same order as in [79], with repsect to various densities of the matrix Q. Since our approach is quite different from the branch-and-cut algorithm employed in the reference, it is difficult to compare the performance of the two approaches directly. To at least give some idea of the performance of our approach relative to that of the reference, we highlight two columns in the tables: the second column, labeled by “LPcnt”, giving the total number of LPs solved in each instance and the third column, labeled by “’time’, giving the computational time for that instance. In these two columns, the results from the reference are labeled by “VN”. The next three columns are labeled by “cnt-dual”, “cnt-M”, and “cnt-rlx”, reporting respectively the number of three types of LPs: those used to generate the ray cuts ($\varphi_0(z)$)or point cuts ($\varphi(z)$), and those (4.30) solved in the sparsification step. The first column in Tables 4.1–4.4 lists the number of satisfiability problems solved in each run. In addition to the total computational time required for each instance, we also report, in the last column labeled by “Gtime”, the amount of time in seconds when a global optimal solution is obtained, but its global optimality is not yet verified. This optimal solution is usually obtained in the local search procedure at the beginning of the runs, but its global optimality is verified only when the algorithm terminates. Comparing the second and last column, we note that the bulk of computations lies in the latter verification step. Notice that among this set of problems, there is only one in the last row of Table 4.2 that could not be solved/verified to global optimality after 10000 iterations; this problem is also not solved by the branch-and-cut approach in [79].

Considering that the LPs in our approach are quite different from those solved in the VN approach, comparing the performance of the these two approaches by counting the numbers of the LPs is not completely fair. However, by setting aside this difference, we can still draw some informative observations about the two approaches. First, the numbers of LPs solved in our approach are quite reasonable and indeed less than the VN numbers in many cases. To be fair, we should note that our approach appears to be more difficult relative to the VN approach (with higher number of LPs) for the problems that require significantly more computational work (e.g., the 7th problem in Table 4.1, the 10th, 16th, 19th, and 20th problem in Table 4.2, etc.); this suggests that there is room for improvement in our approach. Another interesting observation from these tables is that as the sizes of the QP increase, there are more problems that solve less LPs in our approach than the VN approach. Specifically, on problems with 30 variables (Table 4.1), there are 8 out of 15 problems where our approach solve less LPs; on problems with 40 variables (Table 4.2), there are 14 out of 24 problems to our favor; on problems with 50 variables, this fraction increases to 5 out of 6; and finally, on the last set of 3 problems with 60 variables, our approach solves less LPs than the VN approach.

Tables 4.5–4.7 report the computational results for bounded-variable QPs (4.31) with one additional inequality. These tables have the same columns as the previous tables, except for the absence of the VN results. In these tables, the stared problems have the last constraint not binding. The rest of the problems have the inequality constraint biding. Our LPCC approach is able to solve all of the problems presented in the tables to global optimality, which includes two tasks: obtain the optimal solution and verify its global optimality. The problems reported in each table have the same size of variables and are listed in the same order as in the corresponding table reporting the resutls of the bounded-variable QPs. Note that Table 4.6 contains only 9 instances, which have the same data as the first 9 problems listed in Table 4.2. Similarly, the problems listed in Table 4.7 have the same data as the first 3 problems listed in Table 4.3. By comparing the results for the same problems with and without the last constraint, we see that the computational effort increases for the problems with one additional constraint. We suspect two possible reasons for this increased effort: one lies in the sparsification step, in which we have not attempted similar fixings of variables like what we have done in tightening the relaxed LPs (4.30) for the set of bounded-variable QPs. The other reason is that the cuts derived for the MIP problem are probably not as strong as they should be. Of course, the binding or not binding of the additional constraint doubles the number of disjunctions, therefore increasing the complexity of the problem.

Tables 4.8 and 4.9 contain the results for the first set of nonnegatively constrained, copositive, unbounded QPs, for which the existence of stationary solution is not guaranteed. These two tables report the results for two group of problems with 40 and 50 variables, respectively, and 10 randomly generated problems in each group. The algorithm implemented for these QPs does not have the sparsification procedure. Thus the number of relaxed LPs is not reported in these two tables. The number of the LPs reported in the third column is the sum of the fourth and the fifth columns. Since the algorithm is stopped whenever a negative objective value is obtained, we omitted the column "Gtime" in these tables too. From the results, we can tell that for 19 out of 20 problems, our approach is able to identify the unboundedness of the QP. Only one problem, marked with an asterisk sign, does not terminate with a certificate of unboundedness after 20,000 iterations. Tables 4.10 and 4.11 contain the results for the second set of nonnegatively constrained, copositive, unbounded QPs that are guaranteed to have stationary solutions. Interestingly, this second group of QPs seems to be easier to solve than the first group of QPs where stationary solutions are not guaranteed to exist.

As a final comment, we note that in most of the problems solved in the experiments, the numbers (cnt-dual) of ray cuts are significantly more than the numbers (cnt-M) of point cuts. This suggests that there are many infeasible LP pieces in these QPs.

iter	time		LPcnt		cnt-rx	cnt-dual	cnt-M	Gtime
	ours	VN	ours	VN				
233	20.14	22.86	2102	1772	1211	867	24	0.14
3	1.69	1.07	115	55	112	1	2	0.06
83	7.72	15.39	688	1185	487	189	12	0.52
739	77.19	109.41	5617	6676	3078	2477	62	0.17
1	6.55	4.97	304	315	300	0	4	0.16
9	5.53	5.33	282	367	263	15	4	2.53
593	120.55	85.10	6500	5151	3393	3091	16	0.38
1	2.19	2.01	105	113	104	0	1	0.01
1	3.80	2.32	143	121	141	0	2	0.05
45	14.83	41.31	706	2327	516	188	2	0.02
98	38.83	19.12	1430	1156	912	516	2	8.08
24	15.47	14.83	603	804	512	89	2	0.02
369	139.23	77.30	4525	4373	2366	2155	4	0.17
633	172.08	80.18	6458	4259	3348	3084	26	0.08
12	16.19	22.92	453	1278	417	31	5	0.50

Table 4.1: Box constrained QPs with $Q \in R^{30\times30}$

iter	time		LPcnt		cnt-rx	cnt-dual	cnt-M	Gtime
	ours	VN	ours	VN				
1	0.69	3.30	100	186	97	0	3	0.11
1	0.97	2.80	102	201	98	0	4	0.28
1	0.78	2.63	89	139	85	0	4	0.22
548	64.05	143.61	4793	6833	2612	2107	74	0.08
1	4.75	13.55	298	668	296	0	2	0.00
534	66.92	140.51	5105	5861	2791	2259	55	0.27
390	68.27	131.60	4073	5414	2297	1750	26	0.17
195	31.53	70.22	2136	3078	1270	850	16	0.25
193	46.67	55.31	2558	2254	1495	1048	15	2.39
2107	1030.47	983.32	27766	20590	14182	13532	52	0.09
11	11.80	14.42	439	568	409	25	5	0.06
1	7.64	10.09	155	350	153	0	2	0.06
321	241.66	229.41	5312	7622	2860	2448	4	0.03
154	73.84	138.00	2389	4490	1432	950	7	0.08
80	41.42	26.86	1300	1081	859	437	4	0.34
1499	1539.22	359.03	23108	9729	11822	11266	20	0.01
347	277.70	515.81	5987	12690	3152	2830	5	0.11
54	51.59	117.31	928	3687	728	195	5	1.58
751	822.59	199.48	12447	6246	6299	6135	13	0.08
834	833.92	241.00	12558	7202	6407	6126	25	0.33
164	171.83	73.32	2961	2589	1662	1296	3	0.02
1016	2551.34	263.61	21542	7190	10806	10732	4	0.17
3517	6941.48	2169.80	57002	27928	28448	28538	16	0.02
10001*	32206.74	58.84%	184690	36207	91458	93218	14	−−

Table 4.2: Box constrained QPs with $Q \in R^{40\times 40}$.
The problem with the asterisk sign cannot be solved within 10000 iterations.

iter	time		LPcnt		cnt-rx	cnt-dual	cnt-M	Gtime
	ours	VN	ours	VN				
1	4.11	13.28	263	434	260	0	3	0.23
221	27.63	127.07	2065	4285	1286	731	48	1.92
146	18.73	87.91	1375	2827	936	405	34	0.05
1436	703.14	464.57	19833	11356	10250	9523	60	0.02
669	276.28	455.61	8803	10561	4734	4027	42	0.38
288	163.03	263.06	5464	6464	2977	2480	7	0.02

Table 4.3: Box constrained QPs with $Q \in R^{50\times 50}$

iter	time		LPcnt		cnt-rx	cnt-dual	cnt-M	Gtime
	ours	VN	ours	VN				
311	16.53	101.89	1599	2781	1014	446	139	0.11
1	2.13	18.04	109	490	106	0	3	0.08
652	53.50	141.46	3526	3876	1988	1286	252	0.59

Table 4.4: Box constrained QPs with $Q \in R^{60\times 60}$

iter	time	LPcnt	cnt-rx	cnt-dual	cnt-M	Gtime
1072	241.95	11898	6073	5799	26	1.95
347	47.61	3715	1944	1765	6	0.01
967	370.36	13419	6703	6709	7	0.01
2071*	576.13	21420	10788	10561	71	3.84
859	244.27	11355	5607	5741	7	0.02
941	306.75	12847	6415	6424	8	0.08
2063	790.72	24464	12091	12350	23	0.17
331	77.31	3551	1944	1592	15	4.05
1169	333.17	12925	6447	6453	25	2.25
819	342.28	10541	5367	5165	9	0.01
2561	1307.06	33406	16251	17128	27	0.25
894	418.70	12068	6107	5952	9	0.01
1958	1177.31	25854	12671	13165	18	0.05
3383	2181.01	38592	18961	19583	48	4.91
924	456.47	11535	5806	5717	12	448.20

Table 4.5: Box constrained QPs with one additional inequality constraint; $Q \in R^{30\times 30}$**.** The starred problem has the last constraint NOT biding.

iter	time	LPcnt	cnt-rx	cnt-dual	cnt-M	Gtime
1*	2.42	136	132	0	4	0.05
1700	535.91	19931	10002	9902	27	18.33
30	9.36	712	509	202	1	0.00
2309*	1034.20	28918	14603	14256	59	0.20
5619	4563.66	70422	34623	35741	58	1.05
5486	6878.78	78040	38870	39144	26	6233.50
3100	1933.02	41100	20673	20383	44	1831.11
2757	2719.78	40506	20146	20342	18	2.23
4319	7410.64	60421	30228	30167	26	0.11

Table 4.6: Box constrained QPs with one additional inequality constraint; $Q \in R^{40\times 40}$ with density 30%, 40% and 50%. The starred problems have the last constraint NOT biding.

iter	time	LPcnt	cnt-rx	cnt-dual	cnt-M	Gtime
1	11.55	405	405	0	0	0.05
5514	8064.56	81402	41081	40286	35	0.02
2975	4295.75	48139	24276	23855	8	0.31

Table 4.7: Box constrained QPs with one additional inequality constraint; $Q \in R^{50\times50}$ with density 30%.

iter	time	LPcnt	cnt-dual	cnt-M
10455	4989.36	106623	106568	55
11883	7693.13	147875	147849	26
8588	4531.78	115280	115271	9
1361	83.95	15038	15026	12
8569	4343.67	104614	104605	9
11209	6554.17	127020	126927	93
1235	77.69	15910	15910	0
472	15.73	5603	5602	1
302	7.89	3856	3856	0
15605	15064.80	185690	185674	16

Table 4.8: Copositive QPs: $Q \in R^{40\times40}$**, density 0.25, stationary solution not guaranteed.**

iter	time	LPcnt	cnt-dual	cnt-M
17091	17047.94	207155	207101	54
12067	6951.44	137896	137836	60
13483	6991.08	146942	146775	167
7679	3657.99	112001	112001	0
5211	1319.44	67054	67039	15
9664	4845.31	118386	118347	39
14364	12076.95	181824	181809	15
20001*	32815.06	267400	267398	2
1170	81.70	18649	18649	0
468	14.03	6885	6885	0

Table 4.9: Copositive QPs: $Q \in R^{50\times50}$**, density 0.15, stationary solution not guaranteed.** The problem with the asterisk sign can not be solved within 20000 iterations.

iter	time	LPcnt	cnt-dual	cnt-M
829	7.22	2339	2317	22
3854	206.17	16007	15973	34
2931	91.52	9936	9865	71
2115	60.73	10463	10414	49
1207	13.61	3965	3836	129
15059	1844.61	48711	48662	49
656	6.38	2463	2428	35
2768	111.47	12027	11996	31
663	6.78	2533	2517	16
9333	1008.80	39765	39722	43

Table 4.10: Copositive QPs: $Q \in R^{40\times40}$, density 0.25, stationary solution guaranteed

iter	time	LPcnt	cnt-dual	cnt-M
2736	118.99	16242	16162	80
9805	2566.11	68836	68781	55
814	14.06	5019	4862	157
10168	1892.77	59116	59063	53
16618	3877.95	70189	70115	74
10832	2413.30	68483	68373	110
4285	402.17	30691	30628	63
7024	917.91	43321	43262	59
2285	126.81	14319	14298	21
5925	619.39	31346	31270	76

Table 4.11: Copositive QPs: $Q \in R^{50\times50}$, density 0.25, stationarity guaranteed.

CHAPTER 5
SUMMARY

A linear program with linear complementarity constraints plays the same important role in the studies of MPECs as a linear program does in convex programs in addition to many direct applications of its own. Since an LPCC is a special case of an MPEC, many existing computational methods for solving MPECs can be applied to solve LPCCs, including regularization and active set methods. Yet these methods have invariably focused on obtaining a stationary solution that is not guaranteed to be globally optimal for the LPCC. Particularly impressive among these methods are those state-of-art nonlinear programming based solvers which do not rely on the existence of an interior point, such as FILTER which has been used as a benchmark in our computational experiments. One method to globally resolve an LPCC is to introduce a large parameter "big-M", reformulate the LPCC as a mixed-integer problem, and apply various integer programming based techniques to the problem. The deficiency of such an approach is that it assumes the existence of this conceptual parameter "big-M"; in other words, this method is only applicable to the LPCCs that attain finite optimal solutions. A major contribution of this dissertation lies in the parameter-free integer-programming based cutting-plane algorithm presented in Chapter 3 for globally resolving a general LPCC; that is, our method is capable of determining the following three states of an LPCC with valid certificates: the LPCC is infeasible, the LPCC is feasible and unbounded, or the LPCC is optimally solvable. In addition, our algorithm is able to determine on which piece the objective is unbounded for the second case; or compute a global optimal solution of the LPCC for the last case.

The remaining of this dissertation is focused on indefinite quadratic programming, which forms an important application of the LPCCs. This is one of the most important subjects in mathematical programming, playing an essential role in nonlinear programming in addition to many of its own direct applications. There is now an extensive list of literature devoting to this subject; much of which is based on nonlinear programming techniques and the computed solutions are generally stationary points only. The algorithms developed for globally resolving QPs have invariably preassumed that its solvability, that is the QP is known in advance to attain a finite optimal solution. The research on the global resolution of indefinite QPs which are not known *a priori* to be bounded or unbounded on their feasible regions, still remains unresolved until now. It is well known that the QP with finite optima can be resolved by solving an equivalent LPCC reformulation. Inspired by this approach, we have proposed an LPCC approach that is able to identify the QPs which have unbounded objective values on the feasible regions. In this approach, an LPCC is formulated based on the given QP and the global resolution of this LPCC is able to provide a valid certificate of the unboundedness of the QP.

This dissertation consists of several fairly independent chapters. Chapter 2 provides a short review of numerous applications of LPCCs in science, engineering and finance. We have briefly described each application and defined the mathematical formulation for each problem. Although there still exist many other applications arising from different areas, we hope that this short summary will at least give a basic idea of why LPCCs are receiving more attention in mathematical programming, and hope that these efforts can stimulate further research on this subject.

In Chapter 3, we have presented a parameter-free IP based algorithm (Section 3.4) for the global resolution of an LPCC and reported computational results (Section 3.5) obtained from the application of the algorithm for solving a set of randomly generated LPCCs of moderate sizes. The results show that our algorithm is able to successfully identify infeasible or unbounded LPCCs, and also compute the globally optimal solutions of the LPCCs if they exist. Continued research may be conducted on refining the algorithm. For instance, it is found from the experiments that much of the computational efforts were consumed on solving the LPs in the sparsification step. Thus a possible refinement is to find ways to sparsify a cut with more efficiency; in other words, can the sparsification step be implemented without solving too many LPs? Moreover, the algorithm can be applied to realistic classes of LPCCs, such as the bilevel machine learning problems described in [10, 43, 42] and many other practical problems described in Chapter 2. The detailed applications should be explored.

In Chapter 4, we have investigated an LPCC approach to the global resolution of indefinite, possibly unbounded quadratic programs. The main contributions of this research are as follows. First of all, we have introduced an LPCC whose global resolution will certify whether or not the QP attains finite optima (Theorem 13 and Corollary 14). Secondly, we have identified some valid inequalities for the MIP formulation of the LPCC which is an equivalent formulation of a solvable QP. These inequalities, which are motivated by the second-order optimality conditions of the QP (Proposition 16), are expected to improve the efficiency of the LPCC approach. Moreover we have described a new algorithm for solving box-constrained QPs (Subsection 4.4.1). Computational results have been shown to support the promise of the LPCC approach to indefinite QPs (Section 4.5). These are all positive contributions to the study of indefinite QPs. Yet this research is just the first step in developing a general algorithm for globally resolving non-convex QPs; in particular, further study is needed to understand better about the LPCC (4.9) and its MIP formulation, in order to derive deeper cuts and sharper LP relaxations in the sparsification of these cuts.

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