BILEVEL LINEAR PROGRAMS: GENERALIZED MODELS FOR THE LOWER-LEVEL REACTION SET AND RELATED PROBLEMS

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Bilevel programming forms a class of optimization problems that model hierarchical relation between two independent decision-makers, namely, the *leader* and the *follower*, in a collaborative or conflicting setting. Decisions in this hierarchical structure are made sequentially where the leader decides first and then the follower responds by solving an optimization problem, which is parameterized by the leader's decisions. The follower's reaction, in return, affects the leader's decision, usually through shaping the leader's objective function. Thus, the leader should take into account the follower's response in the decision-making process.

A key assumption in bilevel optimization is that both participants, the leader and the follower, solve their problems optimally. However, this assumption does not hold in many important application areas because: (i) there is no known efficient method to solve the lower-level formulation to optimality; (ii) the follower either is not sufficiently sophisticated or does not have the required computational resources to find an optimal solution to the lower-level problem in a timely manner; or (iii) the follower might be willing to give up a portion of his/her optimal objective function value in order to inflict more damage to the leader.

This dissertation mainly focuses on developing approaches to model such situations in which the follower does not necessarily return an optimal solution of the lower-level problem as a response to the leader's action. That is, we assume that the follower's reaction set may include both exact and inexact solutions of the lower-level problem. Therefore, we study a generalized class of the follower's reaction sets. This is arguably the case in many application areas in practice, thus our approach contributes to closing the gap between the theory and practice in the bilevel optimization area.

In addition, we develop a method to solve bilevel problems through single-level reformulations under the assumption that the lower-level problem is a linear program. The most common technique for such transformations is to replace the lower-level linear optimization problem by its KKT optimality conditions. We propose an alternative technique for a broad class of bilevel linear integer problems, based on the strong duality property of linear programs and compare its performance against the current methods. Finally, we explore bilevel models in an application setting of the pediatric vaccine pricing problem.

Keywords: Bilevel optimization, Mixed integer programming, Follower's reaction set, Optimistic bilevel optimization, Pessimistic bilevel optimization, Single-level reformulations.

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PREFACE

First, I would like to thank my advisor, Professor Oleg A. Prokopyev. This work would not had been possible without his support and guidance. I would like to extend my acknowledgement to my committee members, Drs. Osman Y. Özaltın, Denis Sauré, Bo Zeng and Jayant Rajgopal for their time and their constructive feedbacks.

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1.0 INTRODUCTION

The decision-making processes in many practical settings are carried out through a hierarchical interaction between two or more autonomous parties. While they work toward their own objectives in a collaborative or a competitive fashion, each participant's action influences the other's decisions. Bilevel programming models such hierarchical processes between two independent decision-makers, namely, the leader and the follower, and provides a flexible framework to model decentralized decision-making in Stackelbergh games [31, 108] and many important application domains. These areas include transportation [60], energy [15], interdiction [101, 111], military [27], revenue management [40], cybersecurity [7], computational biology [28, 92] and defense [27]. For more details on bilevel optimization we refer the reader to [38] and the references therein.

The decisions in bilevel programs are performed sequentially in which the leader, the upper-level decision-maker, decides first. Consequently, to attain the best response, the follower or the lower-level decision maker, solves an optimization problem which is parameterized by the leader's decision. This setting suggests that, while the leader is able to act strategically by anticipating the follower's (optimal) reaction, the follower's role is rather reactionary. The follower's response, on the other hand, affects the leader's decision, mainly through shaping the leader's objective function and/or constraints. Thus, the leader should always take into account the follower's response in the course of decision-making process.

There are two approaches for modeling the follower's response in bilevel programs [38]: the *optimistic* formulation assumes that if there are multiple optimal solutions to the lower-level problem for a given decision by the leader, then the follower selects the solution that is the most favorable for the leader. On the contrary, the *pessimistic* formulation assumes that the follower selects the least favorable solution for the leader. One should note that in the case of max-min (or min-max) problems optimistic and pessimistic cases coincide.

These two approaches can be generalized via strong-weak bilevel problems [1, 31, 115], where the leader's objective function is a convex combination of the leader's objective functions in the optimistic and pessimistic problems. Thus, the corresponding coefficients in the leader's objective function can be interpreted as the probabilities of cooperation or non-cooperation of the follower, respectively.

A key assumption in bilevel optimization is that both the leader and follower have the computational means to solve the upper- and lower-level formulations optimally, respectively. However, in many important application areas, one has that either: (*i*) there is no known efficient method to solve the lower-level formulation to optimality (for a given set of upper-level decisions); or (*ii*) the follower either is not sufficiently sophisticated or does not have the computational resources necessary to find an optimal solution to the lower-level problem in a timely manner. In both cases, the follower typically resorts to using computationally-tractable heuristic/approximate algorithms. Moreover, the follower might be willing to give up a portion of his[1] optimal objective function value, i.e., select a suboptimal solution in order to inflict more damage to the leader. Such situations may arise in adversarial and interdiction settings where the objectives of the leader and the follower are conflicting, e.g., military and law-enforcement applications. Thus, the leader should be more conservative or guarded when she faces the follower in such situations.

This dissertation mainly focuses on developing approaches to model situations in which the follower does not necessarily return an optimal solution of the lower-level problem as a response to the leader's action. That is, we assume that the follower's reaction set may include both exact and inexact solutions of the lower-level problem, and thus, we study a generalized class of the follower's rational reaction sets. This is arguably the case in many application areas in practice, thus this work contributes to closing the gap between the theory and practice in the bilevel optimization area.

[1] In the remainder of the dissertation we use "her" and "his" whenever we refer to the leader and the follower, respectively.

The remainder of this dissertation is organized as follows. In Chapter 2, we consider a class of bilevel linear mixed-integer programs (BMIPs), where the follower may be willing to give up a portion of his optimal objective function value, and thus may select a suboptimal solution, in order to inflict more damage to the leader. To handle such adversarial settings we consider a modeling approach referred to as α-pessimistic BMIPs. The proposed method naturally encompasses as its special classes pessimistic BMIPs and max-min (or min-max) problems. Furthermore, we extend this new modeling approach by considering strong-weak bilevel programs, where the leader is not certain if the follower is collaborative or adversarial, and thus attempts to make a decision by taking into account both cases via a convex combination of the corresponding objective function values.

In Chapter 3, we study a broad class of bilevel optimization problems where the follower might not react optimally to the leader's actions. In particular, we present an approach in which the leader considers that the follower might use one of a number of known algorithms to solve the lower-level problem either approximately or heuristically. We assume that the leader does not know upfront the algorithm to be used by the follower, but knows that it belongs to a known finite set of algorithms. Thus, the leader is enabled to hedge against the follower's use of suboptimal solutions. In addition, we study the impact of incorporating this realistic feature through numerical experiments in the context of the defender-attacker problem.

A typical method to solve bilevel programs, including those presented in Chapters 1 and 2, is to replace the lower-level problem by Karush-Kuhn-Tucker (KKT) optimality conditions and reformulate it as a single-level problem. This technique is basically applied if the lower-level optimization problem is convex, e.g., a linear program. Alternatively, one can attempt applying the strong duality (SD) property of linear programs to perform such a transformation. In Chapter 4, we exploit this idea for BMIPs where the upper-level variables are integers. Specifically, we describe two SD-based reformulations and compare the performance of an off-the-shelf MIP solver with these reformulations against the KKT-based one.

Furthermore, in Chapter 5, we explore bilevel models in the application setting of the pediatric vaccine pricing problem. We consider a bilevel model of this problem where a vaccine manufacturer (the leader) controls the prices of a set of vaccines and a healthcare provider (the follower) decides whether to purchase a vaccine from the manufacturer or his/her competitors. Assuming that the competitors' prices are not known exactly and are given by an uncertainty set, we present different robust bilevel formulations of this pricing problem. We describe an exact solution approaches for this class of problems.

Finally, Chapter 6 concludes the dissertation and presents our final remarks. We also outline promising directions for future research.

2.0 ON A CLASS OF BILEVEL LINEAR MIXED-INTEGER PROGRAMS IN ADVERSARIAL SETTINGS

2.1 INTRODUCTION

In this chapter we focus on a broad class of bilevel linear mixed-integer programs (BMIPs):

$$
\begin{aligned}
[\mathbf{BMIP}]: \quad & \text{“}\max_{x}\text{”} \quad c^\top x + d_1^\top y \\
& \text{subject to} \quad x \in \mathbb{X}, \\
& \qquad y \in \operatorname*{argmax}_{y} \quad d_2^\top y \\
& \qquad\quad \text{subject to} \quad Ax + By \le h, \\
& \qquad\qquad y \in \mathbb{R}_+^{n_2},
\end{aligned}
$$

where $\mathbb{X} \subseteq \mathbb{Z}_+^{n_1-k} \times \mathbb{R}_+^k$, $A \in \mathbb{R}^{m_2 \times n_1}$, $B \in \mathbb{R}^{m_2 \times n_2}$, $h \in \mathbb{R}^{m_2}$, $c \in \mathbb{R}^{n_1}$, $d_1 \in \mathbb{R}^{n_2}$ and $d_2 \in \mathbb{R}^{n_2}$. The leader's and the follower's decisions variables are denoted by x and y, respectively. The leader's problem is a linear mixed-integer program (MIP).

In the remainder of this chapter we make the following assumptions that are relatively standard in the bilevel optimization literature:

A1: $\mathbb{X} \neq \emptyset$ and $\mathbb{X} = \widehat{\mathbb{X}} \cap \left(\mathbb{Z}_+^{n_1-k} \times \mathbb{R}_+^k\right)$, where $\widehat{\mathbb{X}}$ is a polytope.

A2: For every feasible leader's decision $x \in \mathbb{X}$ the corresponding follower's feasible set is non-empty, i.e., $\{y \in \mathbb{R}_+^{n_2} : \; By \le h - Ax\} \neq \emptyset$ for any $x \in \mathbb{X}$, and bounded.

Following the notation used in some of the bilevel optimization literature [42], we use "max" (with quotes) in the leader's objective function of BMIP to emphasize that there are two possible cases of the bilevel program. Indeed, the pessimistic formulation of **BMIP** is given by:

$$[\mathbf{BMIP}^{\text{pes}}] \quad \max_{x \in \mathbb{X}} \left\{ c^\top x + \min_{y \in H(x)} d_1^\top y \right\}, \tag{2.1}$$

$$\text{where } H(x) = \operatorname{argmax}\{d_2^\top y : \; Ax + By \le h, \; y \in \mathbb{R}_+^{n_2}\}, \tag{2.2}$$

and $H(x)$ denotes the *lower-level (follower's) rational reaction set* for a given x. Note that (2.1) involves a minimization problem over optimal solutions of the follower's problem for a given leader's decision.

On the other hand, the optimistic **BMIP** is formulated by simply eliminating the min operator from the objective function (2.1) that is:

$$[\mathbf{BMIP}^{\text{opt}}] \quad \max_{x \in \mathbb{X}, \; y \in H(x)} c^\top x + d_1^\top y \tag{2.3}$$

Given the leader's decision x, we denote by $f(x)$ and $f^p(x)$ the optimistic and pessimistic objective function values of the leader, respectively. Similarly, we denote by f^* and f_p^*, the *optimal* objective function values of the leader in the *optimistic* and *pessimistic* cases, respectively.

Note that if $k = n_1$, then **BMIP** reduces to a bilevel linear program (BLP). Bilevel programming, in particular, BMIPs and BLPs, where for a given leader's decision the corresponding follower's problem reduces to a linear program (LP) as in (2.2), is a well-studied area of optimization with a host of algorithmic and theoretical developments; see, e.g., [8, 10, 12, 38, 41]. In particular, it is known that, in contrast to polynomially solvable single-level LPs, BLPs are NP-hard optimization problems [46]. Furthermore, due to the fact that the follower's problem in (2.2) is an LP, BMIPs can be reformulated as single-level linear MIPs [9], which consequently can be solved either via standard MIP solvers or by using some specialized approaches [10, 38, 41]. Bilevel problems that involve integrality restrictions for the follower's variables, see, e.g., some recent results in [34, 45, 104], are outside the scope of this chapter.

In view of the brief discussion above, our contributions in this chapter are as follows:

• First, we consider computational complexity of BLPs in the context of optimistic and pessimistic solutions (see Section 2.2). In particular, we establish that even if an optimal optimistic (or pessimistic) solution to BLP is known, then the problem of finding an optimal pessimistic (or optimistic) solution to the same BLP remains an NP-hard problem. Moreover, we show that even if one of the optimal solutions (either pessimistic or optimistic) to BLP is known, then it is still an NP-hard problem to identify a leader's solution that is, first, optimal for both optimistic and pessimistic BLPs, and, second, provides the same objective function value in both cases (if such solution exists).

• Second, we propose a generalization of pessimistic BMIPs, where the follower might willingly give up a portion of his optimal objective function value, and thus select a suboptimal solution in order to inflict more damage to the leader (see Section 2.3). We refer to our proposed models as α-*pessimistic* BMIPs, where parameter α controls the sub-optimality level of the follower and mimics constant-factor approximation ideas that are often used in the literature, see, e.g., [54, 106]. Clearly, such situations may arise in adversarial and interdiction settings, e.g., military and law-enforcement applications, which is the main motivation behind this study. (We illustrate our results with an example of the defender-attacker problem in Section 2.5.2.) Thus, the leader should be more conservative or guarded when faces a follower that is α-suboptimal. Our model naturally encompasses as its special classes both pessimistic BMIPs and max-min (or min-max) problems. In particular, for $\alpha = 1$ the proposed approach corresponds to pessimistic BMIPs, while the case of $\alpha = 0$ reduces α-*pessimistic* BMIPs to max-min problems. The latter corresponds to the worst-case scenario for the leader, where the follower completely disregards his objective function and is focused on disrupting the leader's performance. Therefore, the proposed model can be viewed as an approach for the leader to balance her level of conservatism through the value of parameter α in adversarial settings where the leader is not completely confident regarding the follower's commitment to his objective function. We refer the reader for more detailed discussion on these issues in Section 2.3. We study the structural properties of α-pessimistic BMIPs and illustrate its relationships with optimistic and pessimistic BMIPs.

• Third, we incorporate the proposed model of a sub-optimal adversarial follower into the context of *strong-weak* BMIP models [1, 31, 119], which is an extension of the ideas behind optimistic and pessimistic BMIPs (see Section 2.4). Specifically, in a strong-weak approach we model a partially collaborative follower by assuming that the leader's objective function is a convex combination of the leader's objective functions in the optimistic and pessimistic cases. Furthermore, the coefficients in this summation can be interpreted as the probabilities of cooperation or non-cooperation of the follower, respectively. That is, the leader is not certain if the follower is either collaborative or adversarial, and thus attempts to make a "robust" decision by taking into account both situations. Our approach, referred to as the *strong-α-weak* model, can be viewed as a natural generalization of the strong-weak model from [31, 119] as it assumes that the follower may be α-pessimistic, which allows us to consider more general types of adversarial followers including those that completely disregard their objective functions. Thus, our approach naturally links optimistic, pessimistic and max-min models within a unified framework. Another related question when comparing the strong-α-weak model against either purely optimistic or pessimistic cases of BMIP is that how much the decision-maker (i.e., the leader) "loses" in terms of the obtained objective function value if the follower is, in fact, either optimistic or α-pessimistic, respectively. In Section 2.4 we derive some bounds for such "losses."

Finally, in Section 2.5 we consider an application of BMIPs, namely, a class of defender-attacker models. We illustrate our theoretical results from Sections 2.3 and 2.4 with numerical examples and provide some insights into the links between optimistic, pessimistic and strong-weak modeling approaches.

2.2 COMPUTATIONAL COMPLEXITY: OPTIMISTIC VS. PESSIMISTIC CASES

It is well-known that any linear mixed 0–1 programming problem can be reduced to a BLP instance [9]. Therefore, BLPs are strongly NP-hard [61]. We refer the reader to [46], which provides a brief survey on computational complexity of BLPs, in particular, with respect to issues related to polynomially solvable classes of the problem and inapproximability results.

BLPs are among the simplest classes of bilevel programs, which implies that the computational complexity results established in this section hold for more general bilevel optimization problems. Specifically, our main focus is on the following research questions:

- If the decision-maker knows an optimistic (pessimistic) solution to a BLP, does it simplify the problem of finding a pessimistic (optimistic) solution to the same BLP?
- How difficult is it to identify a leader's solution that is optimal to both optimistic and pessimistic cases (assuming that such solution exists) when one of the optimal solutions (either pessimistic or optimistic) is known?

In our derivations below we exploit the **SUBSET SUM** problem that is known to be NP-complete [54].

SUBSET SUM: Given a set of positive integers $S = \{s_1, s_2, \ldots, s_n\}$, and a positive integer K, does there exist a subset $S' \subseteq S$ such that $\sum_{i:\ s_i \in S'} s_i = K$?

Next, consider the following BLP instance:

$$
\begin{aligned}
\text{“}\min_{x}\text{”} \quad & \sum_{i=1}^{n} s_i x_i + K x_{n+1} + \sum_{i=1}^{n} v_i + M u && \text{(2.4a)}\\
\text{s.t.} \quad & \sum_{i=1}^{n} s_i x_i + K x_{n+1} \geq K, && \text{(2.4b)}\\
& 0 \leq x_i \leq 1, \quad i = 1, \ldots, n+1, && \text{(2.4c)}\\
& (v, u) \in \operatorname*{argmax}_{v,u} \quad \sum_{i=1}^{n} v_i + (u - v_{n+1}) && \text{(2.4d)}\\
& \qquad \text{s.t.} \quad v_i \leq 1 - x_i, \qquad i = 1, \ldots, n, && \text{(2.4e)}\\
& \qquad \qquad v_i \leq x_i, \qquad i = 1, \ldots, n, && \text{(2.4f)}\\
& \qquad \qquad 0 \leq u \leq x_{n+1}, && \text{(2.4g)}\\
& \qquad \qquad u - v_{n+1} \leq 1 - x_{n+1}, && \text{(2.4h)}\\
& \qquad \qquad u - v_{n+1} \leq x_{n+1}, && \text{(2.4i)}\\
& \qquad \qquad v_i \geq 0, \quad i = 1, \ldots, n+1. && \text{(2.4j)}
\end{aligned}
$$

where M is a sufficiently large positive constant parameter.

Lemma 1. *The following statements hold for model (2.4):*

(i) $x^* = (0, \ldots, 0, 1)^\top$, $u^* = v_1^* = \ldots = v_{n+1}^* = 0$ *is an optimal optimistic solution, and* $f^* = K$.

(ii) $f_p^* = K$ *iff the answer to the considered instance of the* ***SUBSET SUM*** *problem is "yes."*

(iii) there exists a leader's decision x^* *such that* $f^* = f(x^*) = f^p(x^*) = f_p^* = K$*, i.e.,* x^* *is optimal for both optimistic and pessimistic cases, iff the answer to the considered instance of the* ***SUBSET SUM*** *problem is "yes."*

Proof.

(i) Observe that $f^* \geq K$ due to (2.4b). Then it is easy to check that $x_1^* = \ldots = x_n^* = 0$, $x_{n+1}^* = 1$, and $u^* = v_1^* = \ldots = v_{n+1}^* = 0$ is an optimal optimistic solution with $f^* = K$.

(ii) $\Longleftarrow$ Suppose the answer to the **SUBSET SUM** problem is "yes." Consider the leader's solution, where $\bar{x}_{n+1} = 0$, and $\bar{x}_i = 1$ if $s_i \in S'$ or $\bar{x}_i = 0$, otherwise, for $i = 1, \ldots, n$. From (2.4e), (2.4f) and (2.4g), $\bar{u} = \bar{v}_1 = \ldots = \bar{v}_n = \bar{v}_{n+1} = 0$ is the respective solution of the follower, and so $f_p^* = K$. $\Longrightarrow$ Let $f_p^* = K$ and $\bar{x}$ be an optimal pessimistic solution of the leader. Then, from (2.4a) and (2.4b), $\bar{u} = \bar{v}_1 = \ldots = \bar{v}_n = 0$. Therefore, $\bar{x}_1 \ldots, \bar{x}_n \in \{0, 1\}$. Note that if $\bar{x}_{n+1} > 0$ then the follower implements the solution that maximizes the leader's objective, that is $\bar{u} = \bar{x}_{n+1} > 0$ and $\bar{v}_{n+1} = \bar{u} - \min\{1 - \bar{x}_{n+1}, \bar{x}_{n+1}\}$, which is a contradiction. Therefore, $\bar{x}_{n+1} = 0$. The required result follows if we let $s_i \in S'$ iff $\bar{x}_i = 1$, $i = 1, \ldots, n$.

(iii) From (ii), $f^* = f_p^* = K$ iff the answer to the **SUBSET SUM** problem is "yes." Note that the same solution of the leader, i.e., $\bar{x}_{n+1} = 0$, and $\bar{x}_i = 1$ if $s_i \in S'$ or $\bar{x}_i = 0$, otherwise, for $i = 1, \ldots, n$, is constructed in both directions of (ii), and this solution is also optimal in the optimistic case. ∎

Note that constraints of the form (2.4e)-(2.4f) are often used for linking lower- and upper-level variables while proving theoretical results in bilevel programming [9, 61]. For example, in [61] such constraints are exploited for showing that linear max-min programs are strongly NP-hard. The main novelty of our reduction is in using constraints of the form (2.4g)-(2.4i) and the corresponding additional terms in the objective functions (2.4a) and (2.4d), which allows us to obtain the following results based on Lemma 1:

Proposition 1. *The problem of finding an optimal pessimistic solution of BLP remains NP-hard even if an optimal optimistic solution of the same BLP is known.*

Proposition 2. *Checking whether there exists leader's decision x^*, that:*
(a) is optimal for both optimistic and pessimistic cases of BLP, and
(b) simultaneously provides the same objective function values for both cases,
is NP-complete even if an optimal optimistic solution is known.

Proposition 3. *Checking whether the BLP has multiple optimal optimistic solutions is NP-hard.*

In order to extend Proposition 1 we also analyze complexity of BLP when an optimal pessimistic solution is known. Consider another instance of BLP given by:

$$\text{“}\min_x\text{”} \quad \sum_{i=1}^{n} s_i x_i + (K+M)x_{n+1} + \frac{2M}{n}\sum_{i=1}^{n}(v_i + u_i) \tag{2.5a}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} s_i x_i + K x_{n+1} \geq K, \tag{2.5b}$$

$$0 \leq x_i \leq 1, \quad i = 1, \ldots, n+1, \tag{2.5c}$$

$$(v,u) \in \operatorname*{argmax}_{v,u} \quad \sum_{i=1}^{n}(u_i - v_i) \tag{2.5d}$$

$$\text{s.t.} \quad u_i - v_i \leq 1 - x_i, \qquad i = 1, \ldots, n, \tag{2.5e}$$

$$u_i - v_i \leq x_i, \qquad i = 1, \ldots, n, \tag{2.5f}$$

$$0 \leq v_i \leq 1 - x_{n+1}, \quad i = 1, \ldots, n, \tag{2.5g}$$

$$u_i \geq 0, \qquad i = 1, \ldots, n, \tag{2.5h}$$

where M is a sufficiently large positive constant parameter.

Another interesting observation from Lemma 1 (i) is given in the following remark.

Remark 1. Consider an instance of BLP given by (2.4) and let the follower be adversarial, while the leader makes a decision $x_1^* = \ldots = x_n^* = 0$, $x_{n+1}^* = 1$ by assuming a cooperative follower, i.e., an optimistic case. In response, the adversarial follower would implement $u = v_{n+1} = 1$. Thus, $f^p(x^*) = K + M$, while $f_p^* = K$ by Lemma 1. Consequently, $f^p(x^*) - f_p^* = M$, which is a positive constant parameter. Therefore, if the leader assumes an optimistic case of BLP, while the follower is adversarial, i.e., the considered BLP is pessimistic, then the difference in the objective function values of the obtained solutions can be arbitrarily large.

Lemma 2. *The following statements hold for model (2.5):*

(i) $\bar{x} = (0, \ldots, 0, 1)^\top$, $\bar{v}_1 = \ldots = \bar{v}_n = \bar{u}_1 = \ldots = \bar{u}_n = 0$ *is an optimal pessimistic solution with* $f_p^* = K + M$.

(ii) $f^* = K$ *iff the answer to the considered instance of the* ***SUBSET SUM*** *problem is "yes."*

Proof.

(i) Let $\bar{x}$ be a feasible solution of the leader with $\bar{x}_{n+1} = 1$. Then, it is optimal for the leader to set $\bar{x}_1 = \ldots = \bar{x}_n = 0$. Thus, $f^p(\bar{x}) = K + M$. Similarly, let $\widetilde{x}$ be a feasible solution of the leader with $0 \leq \widetilde{x}_{n+1} < 1$. Then, in the pessimistic case, the follower can set $v_i = 1 - \widetilde{x}_{n+1}$ for all $i = 1, \ldots, n$, while having (2.5e)-(2.5f) satisfied. Therefore, $f^p(\widetilde{x}) \geq K + M\widetilde{x}_{n+1} + 2M(1 - \widetilde{x}_{n+1}) = K + 2M - M\widetilde{x}_{n+1} > K + M$, which implies the necessary result.

(ii) $\Longleftarrow$ Suppose the answer to the instance of the **SUBSET SUM** problem is "yes." Consider the leader's solution, where $x^*_{n+1} = 0$, and $x^*_i = 1$ if $s_i \in S'$ and $x^*_i = 0$, otherwise, for $i = 1, \ldots, n$. In the optimistic case, the follower sets $u^*_i = v^*_i = 0$ for all $i = 1, \ldots, n$. Thus, $f^* = f(x^*) = K$. $\Longrightarrow$ Let $f^* = K$ and x^* be the corresponding optimal optimistic solution of the leader. Then, from (2.5a) and (2.5b), we conclude that $x^*_{n+1} = 0$ and the follower's optimistic solution is $u^*_1 = \ldots = u^*_n = v^*_1 = \ldots = v^*_n = 0$. Therefore, $x^*_1, \ldots, x^*_n \in \{0, 1\}$. Finally, the required statement follows by setting $s_i \in S'$ iff $x^*_i = 1$, $i = 1, \ldots, n$. ∎

Based on Lemma 2 we immediately obtain the following result:

Proposition 4. *The problem of finding an optimal optimistic solution of BLP remains* NP*-hard even if an optimal pessimistic solution of the same BLP is known.*

Another observation from Lemma 2 is similar in spirit to the earlier remark. Specifically:

Remark 2. Suppose that the follower is collaborative, i.e., BLP is optimistic, but the leader makes a decision $\bar{x}_1 = \ldots = \bar{x}_n = 0$, $\bar{x}_{n+1} = 1$ by assuming an adversary follower, i.e., pessimistic BLP. In response to the leader's decision, the collaborative follower implements $u_i^* = v_i^* = 0$ for all $i = 1, \ldots, n$. Thus, $f(\bar{x}) = K + M$. Assume that the answer to the considered instance of the **SUBSET SUM** problem is "yes." Consequently, $f^* = K$ and $f(\bar{x}) - f^* = M$, which implies that if the leader assumes a pessimistic BLP while the follower is collaborative, then the difference in the objective function values of the obtained solutions can be arbitrarily large.

2.3 SUBOPTIMAL RESPONSE TO THE LEADER'S DECISION: ADVERSARIAL FOLLOWER

Constraint (2.2) requires that the follower always implements one of his optimal solutions in response to each leader's decision. In this section, we consider a more general non-cooperative (adversarial) setting, where the follower, in order to inflict more "damage" to the leader, can give up a portion of his optimal objective function value by selecting a suboptimal solution. Specifically, we propose modeling such settings by defining a suboptimal lower-level reaction set for a given leader's decision x of the following form:

$$H_\alpha(x) = \{y' \in \mathbb{R}_+^{n_2} : \ d_2^\top y' \geq \alpha d_2^\top y + (1-\alpha)L, \ y \in H(x), \ Ax + By' \leq h\}, \tag{2.6}$$

where parameter $\alpha \in [0, 1]$ controls the suboptimality level of the follower. In (2.6) we assume that the follower's objective function is bounded from below by a fixed constant L for any decision of the leader. Then, the pessimistic BMIP generalizes to:

$$[\alpha\text{-}\mathbf{BMIP}^{\text{pes}}] \quad \max_{x \in \mathbb{X}} \left\{c^T x + \min_{y \in H_\alpha(x)} d_1^\top y\right\}, \tag{2.7}$$

which is referred to as α-pessimistic **BMIP**. By comparing (2.1) and (2.7), observe that the α-pessimistic **BMIP** is obtained from the pessimistic **BMIP** by enlarging the follower's reaction set. Specifically, if $y \in H(x)$, then $y \in H_\alpha(x)$ for any $\alpha \in [0, 1]$ due to the assumption on L. Therefore, $H(x) \subseteq H_\alpha(x)$ for any leader's decision $x \in \mathbb{X}$. In general, $H_{\alpha_1}(x) \subseteq H_{\alpha_2}(x)$ for any $\alpha_1 \geq \alpha_2$ and $\alpha_1, \alpha_2 \in [0,1]$. Simply speaking, by introducing set $H_\alpha(\cdot)$, which is a generalization of the lower-reaction set $H(\cdot)$, we allow the follower to have more flexibility than in standard pessimistic BMIPs to select a solution that is more damaging to the leader's objective function value.

One of the main motivations behind the proposed definition of $H_\alpha(\cdot)$ is to mimic constant-factor approximation ideas that are often used in the literature, see, e.g., [54, 106]. For example, the reaction set of the form (2.6) naturally arises when $L = 0$ (e.g., the follower's objective function is non-negative) and the follower applies an α-approximation algorithm instead of an exact method. (In Section 2.4 we exploit such ideas to provide some approximation guarantees in the context of the strong-weak model.)

Our modeling framework allows for two possible interpretations. In the first one, the follower sets the value of α, which is also known to the leader, and optimizes against the leader's objective while also ensuring that his decision achieves α-optimality with respect to his own objective function. In the other interpretation, the follower does not set α, but when making the upper-level decisions, the leader takes into account the case where the follower may select an α-suboptimal solution. Thus, α is set by the leader to make conservative or guarded upper-level decisions in anticipation of the follower's suboptimal response.

Observe that if $\alpha = 1$, then $H_1(x) = H(x)$ and α-pessimistic **BMIP** reduces to standard pessimistic **BMIP**, where the follower responds to the leader's decision optimally. Conversely, if $\alpha = 0$, then the follower completely disregards his own objective function, and merely focuses on minimizing the leader's benefit. In this case, α-pessimistic **BMIP** reduces to a standard max-min problem, where both decision-makers have the same objective function, but their goals are in opposite directions, i.e.,

$$\max_{x \in \mathbb{X}} \left\{ c^\top x + \min_{y \in \mathbb{R}^{n_2}_+} \{ d_1^\top y : Ax + By \leq h \} \right\} \tag{2.8}$$

Max-min problems of the form (2.8) arise in a variety of application domains [38, 81]. For example, the classical shortest path network interdiction problem, see, e.g., [68], is a special class of (2.8), where the leader (interdictor) selects a decision (e.g., removes a set of nodes and/or edges) in order to maximally increase the length of the shortest path for the follower (evader), who travels on a given network between two fixed nodes, i.e., an origin and a destination node.

The discussion above implies that the α-pessimistic **BMIP** contains both the pessimistic **BMIP** and the max-min problem as its special cases, and thus can be viewed as their natural generalization. More importantly, we believe that the proposed modeling approach can be leveraged to address the following issues:

• In adversarial settings the standard max-min approach given by (2.8) is used to provide the worst-case analysis for the decision-maker. This approach is commonly used in the related literature including the defender-attacker, attacker-defender and interdiction models. Such analysis assumes that the follower's sole objective is to disrupt the leader's performance to the maximum possible extent. On the other hand, the proposed α-pessimistic approach allows to capture settings where, in addition to disrupting the leader's objective function the follower has an alternative goal. For example, in the defender-attacker models the follower may want to maximize his probability of survival after the attack. Clearly, he may sacrifice some of this objective in order to inflict more damage to the leader and the parameter α allows the leader to control this trade-off.

• The max-min model given by (2.8) often arises in the symmetric data/information scenarios. For example, in interdiction applications such assumption implies that both the leader and the follower have the same cost parameters. On the other hand, the pessimistic BMIP is capable of modeling more general assymetric scenarios, see, e.g., [17], which, in turn, can be exploited by the leader to improve her objective function value in comparison to the conservative max-min approach that captures the worst-case scenario for the leader. However, in practice the leader may not be completely confident about the objective function of the follower. Thus, the parameter α allows the decision-maker, i.e., the leader, to control her level of conservatism.

• In practice it is also conceivable that the follower may not be a rational decision-maker or have bounded rationality and thus, he may implement a suboptimal solution. The parameter α allows the leader to control her level of conservatism in such cases. Admittedly, the actual value of α may be unknown to the leader. However, by performing the sensitivity analysis with respect to α, the leader can obtain deeper insights into her possible solution strategies. Furthermore, we also explore potential leader's "losses" when α is misspecified, see our further discussion at the end of this section.

Next, we provide some theoretical results in the context of the proposed modeling approach. Let x^* and $\bar{x}^\alpha$ be the leader's optimal solutions in the optimistic (2.3) and α-pessimistic (2.7) **BMIP** formulations, respectively. Given the leader's decision $x \in \mathbb{X}$, let $w(x)$, $y^p(x)$ and $y^\alpha(x)$ be the corresponding follower's decisions in the optimistic, pessimistic and α-pessimistic cases, respectively. Thus, $w(x) \in H(x)$, $y^p(x) \in H(x)$ and $y^\alpha(x) \in H_\alpha(x)$. Also, denote by $f^p_\alpha(x)$ the objective function value of the leader in the α-pessimistic case and let $f^*_\alpha = f^p_\alpha(\bar{x}^\alpha)$. Note that $f^p_1(x) = f^p(x)$ and $f^*_1 = f^*_p$; furthermore, f^*_0 is the optimal objective function value of (2.8).

Proposition 5. *$f^* \geq f^*_p \geq f^p(\bar{x}^\alpha) \geq f^*_\alpha$ for any $\alpha \in [0,1]$.*

Proposition 6. *f^*_α and $f^p_\alpha(x)$ are non-decreasing in $\alpha \in [0,1]$.*

The proofs of the above two propositions are omitted as they hold by the definitions (2.2) and (2.6), which imply that $H(x) \subseteq H_\alpha(x)$.

Proposition 7. *$f^p_\alpha(x)$ is convex in $\alpha \in [0,1]$ for any $x \in \mathbb{X}$.*

Proof. Consider $\alpha = \theta\alpha_1 + (1-\theta)\alpha_2$ for $\theta \in [0,1]$. Let $\widetilde{y} = \theta y^{\alpha_1}(x) + (1-\theta)y^{\alpha_2}(x)$ for $x \in \mathbb{X}$. Observe that $\widetilde{y} \geq 0$ and

$$\begin{aligned} Ax + B\widetilde{y} &= Ax + B\left(\theta y^{\alpha_1}(x) + (1-\theta)y^{\alpha_2}(x)\right) \\ &= \theta\left(Ax + By^{\alpha_1}(x)\right) + (1-\theta)\left(Ax + By^{\alpha_2}(x)\right) \leq \theta h + (1-\theta)h = h. \end{aligned}$$

Furthermore, let $y \in H(x)$. As $y^{\alpha_1}(x) \in H_{\alpha_1}(x)$ and $y^{\alpha_2}(x) \in H_{\alpha_2}(x)$, then:

$$\begin{aligned} d_2^\top \widetilde{y} &= \theta d_2^\top y^{\alpha_1}(x) + (1-\theta) d_2^\top y^{\alpha_2}(x) \\ &\geq \theta\left(\alpha_1 d_2^\top y + (1-\alpha_1)L\right) + (1-\theta)\left(\alpha_2 d_2^\top y + (1-\alpha_2)L\right) = \alpha d_2^\top y + (1-\alpha)L, \end{aligned}$$

which implies that $\widetilde{y} \in H_\alpha(x)$ and $d_1^\top \widetilde{y} \geq d_1^\top y^\alpha(x)$. Therefore:

$$\begin{aligned} f^p_\alpha(x) =& c^\top x + d_1^\top y^\alpha(x) \leq c^\top x + d_1^\top \widetilde{y} = c^\top x + d_1^\top\left(\theta y^{\alpha_1}(x) + (1-\theta)y^{\alpha_2}(x)\right) \\ =& \theta\left(c^\top x + d_1^\top y^{\alpha_1}(x)\right) + (1-\theta)\left(c^\top x + d_1^\top y^{\alpha_2}(x)\right) = \theta f^p_{\alpha_1}(x) + (1-\theta) f^p_{\alpha_2}(x), \end{aligned}$$

which concludes the proof. ∎

Corollary 1. *f^*_α is convex in $\alpha \in [0,1]$.*

Proof. It follows directly from the fact that $\bar{x}^\alpha \in \mathbb{X}$ and $f^*_\alpha = f^p_\alpha(\bar{x}^\alpha)$. ■

Corollary 2. *For $\alpha \in [0,1]$ and $x \in \mathbb{X}$, $f^p_\alpha(x) \le \alpha f^p_1(x) + (1-\alpha) f^p_0(x)$ and $f^*_\alpha \le \alpha f^*_p + (1-\alpha) f^*_0$.*

Next, we define Δ_α as

$$\Delta_\alpha = f^*_\alpha - f^p_\alpha(x^*), \tag{2.9}$$

i.e., the leader's "loss" when she implements optimal optimistic solution x^*, while the follower is α-pessimistic. In other words, the leader can be viewed as "over-optimistic" about the follower's response to her decisions. Clearly, by its definition $\Delta_\alpha \ge 0$. The above properties of α-pessimistic solutions allow us to establish some additional lower and upper bounds on Δ_α.

Proposition 8. *Let $0 \le \alpha_1 \le \alpha_2 \le 1$ and $\alpha = \theta\alpha_1 + (1-\theta)\alpha_2$ for $\theta \in [0,1]$. Then:*

$$\max\left\{0, \theta\Delta_{\alpha_1} + (1-\theta)\Delta_{\alpha_2} - (1-\theta)(f^*_{\alpha_2} - f^*_{\alpha_1})\right\} \le \Delta_\alpha \le \Delta_{\alpha_1} + (1-\theta)(f^*_{\alpha_2} - f^*_{\alpha_1}). \tag{2.10}$$

Proof. Recall that x^* denotes an optimal optimistic solution for the leader. From Propositions 6 and 7:

$$\begin{aligned}\Delta_\alpha =& f^*_\alpha - f^p_\alpha(x^*) \ge f^*_{\alpha_1} - \theta f^p_{\alpha_1}(x^*) - (1-\theta) f^p_{\alpha_2}(x^*)\\ =& \theta\Delta_{\alpha_1} + (1-\theta) f^*_{\alpha_1} - (1-\theta) f^p_{\alpha_2}(x^*) = \theta\Delta_{\alpha_1} + (1-\theta)\Delta_{\alpha_2} - (1-\theta)(f^*_{\alpha_2} - f^*_{\alpha_1}).\end{aligned}$$

Recall that Δ_α is nonnegative by its definition. Thus, the left inequality in (2.10) follows. By using Propositions 6 and Corollary 1, we have the following:

$$\begin{aligned}\Delta_\alpha =& f^*_\alpha - f^p_\alpha(x^*) \le \theta f^*_{\alpha_1} + (1-\theta) f^*_{\alpha_2} - f^p_{\alpha_1}(x^*)\\ =& \Delta_{\alpha_1} - (1-\theta) f^*_{\alpha_1} + (1-\theta) f^*_{\alpha_2} = \Delta_{\alpha_1} + (1-\theta)(f^*_{\alpha_2} - f^*_{\alpha_1}),\end{aligned}$$

which provides the right inequality in (2.10). ■

Corollary 3. *$\Delta_\alpha \le \Delta_0 + \alpha(f^*_p - f^*_0)$ for any $\alpha \in [0,1]$.*

In general, Δ_α is not monotone in α. However, from Propositions 7 and Corollary 1, it follows that Δ_α is equal to the difference of two convex functions, i.e., Δ_α is a d.c. function [65].

Next, for $0 \leq \alpha_1 \leq \alpha_2 \leq 1$ we define $\delta_{\alpha_1,\alpha_2}$ as

$$\delta_{\alpha_1,\alpha_2} = f^*_{\alpha_2} - f^p_{\alpha_2}(\bar{x}^{\alpha_1}), \tag{2.11}$$

i.e., the leader's "loss," who implements optimal α_1-pessimistic solution $\bar{x}^{\alpha_1}$, while the follower is α_2-pessimistic. In other words, the leader can be viewed as conservative and "over-pessimistic" about the follower's response to her decisions. The dependence of $\delta_{\alpha_1,\alpha_2}$ on $\bar{x}^{\alpha_1}$ can be omitted if $\bar{x}^{\alpha_1}$ is either unique or provides the same value of $f^p_{\alpha_2}$ and the latter is assumed below.

Proposition 9. *Let* $0 \leq \alpha_1 < \alpha_2 \leq 1$. *Then*

$$0 \leq \delta_{\alpha_1,\alpha_2} \leq f^*_{\alpha_2} - f^*_{\alpha_1} \leq \frac{\alpha_2 - \alpha_1}{1 - \alpha_1} \cdot \left(f^*_p - f^*_{\alpha_1}\right). \tag{2.12}$$

Proof. By definition $\delta_{\alpha_1,\alpha_2} \geq 0$. Next, from Propositions 5 and 6 along with Corollary 1, we have the following inequalities:

$$\delta_{\alpha_1,\alpha_2} = f^*_{\alpha_2} - f^p_{\alpha_2}(\bar{x}^{\alpha_1}) \leq f^*_{\alpha_2} - f^*_{\alpha_1} \leq \left(\frac{1-\alpha_2}{1-\alpha_1}\right) f^*_{\alpha_1} + \left(\frac{\alpha_2-\alpha_1}{1-\alpha_1}\right) f^*_p - f^*_{\alpha_1} \leq \frac{\alpha_2-\alpha_1}{1-\alpha_1} \cdot \left(f^*_p - f^*_{\alpha_1}\right).$$

■

Corollary 4. $\delta_{0,\alpha} \leq f^*_\alpha - f^*_0$ *and* $\delta_{\alpha,1} \leq f^*_p - f^*_\alpha$ *for any* $\alpha \in [0,1]$.

In this section, we mostly focus on the "max-max" BMIPs, i.e., both the leader's and the follower's optimization problems involve maximization objectives. For other possible cases of BMIPs, the structural results obtained in this section should be modified by simple adjustments, which are rather straightforward in view of the provided derivations.

For example, in the case of "min-max" BMIPs the definition of Δ_α and $\delta_{\alpha_1,\alpha_2}$ should be changed to $\Delta_\alpha = f^p_\alpha(x^*) - f^*_\alpha$ and $\delta_{\alpha_1,\alpha_2} = f^p_{\alpha_2}(\bar{x}^{\alpha_1}) - f^*_{\alpha_2}$, respectively. The corresponding bounds in Propositions 8 and 9 as well as their corollaries can be modified accordingly. Finally, we note that some additional discussion on this issue is also provided in Section 2.5, where we describe an application example of **BMIP** that involve "min-max" problems.

To illustrate some basic properties of α-pessimistic **BMIP** developed in this section, we consider the following example:

$$\max_{\mathbf{x}\in\{0,1\}^2} \quad f(x,y) = 15x_1 + 10x_2 + 2y_1 + y_2 \tag{2.13a}$$

$$\text{subject to} \quad x_1 + x_2 \leq 1, \tag{2.13b}$$

$$\mathbf{y} \in \underset{\mathbf{y}\in\mathbb{R}^2_+}{\operatorname{argmax}}\{y_1 + y_2 \ : \ 3x_1 + 6x_2 \leq y_1 + y_2 \leq 10x_1 + 12x_2, \ y_1 \geq 3x_2\} \tag{2.13c}$$

Observe that in (2.13) the leader has only three feasible actions given in Table 1. The corresponding follower's feasible regions are illustrated in Figure 1. Furthermore, Table 1 provides optimal solutions in the optimistic, pessimistic and α-pessimistic cases, where we assume that $L = 0$ in the definition of $H_\alpha(x)$ given by (2.6).

Table 1: The follower's decisions and the leader's objective function values for each leader's decision. We assume $L = 0$ in (2.6). Note that for $\alpha = 0$, i.e., the max-min problem, the leader implements $\mathbf{x}^3$.

Solution	optimistic		pessimistic		α–pessimistic	
	$\mathbf{w}(\mathbf{x})$	$f(\mathbf{x})$	$\mathbf{y}^p(\mathbf{x})$	$f^p(\mathbf{x})$	$\mathbf{y}^\alpha(\mathbf{x})$	$f^p_\alpha(\mathbf{x})$
$\mathbf{x}^1 = (0,0)^\top$	$(0,0)^\top$	0	$(0,0)^\top$	0	$(0,0)^\top$	0
$\mathbf{x}^2 = (1,0)^\top$	$(10,0)^\top$	35	$(0,10)^\top$	25	$\left\{\begin{array}{l}(0,3)^\top,\\ (0,10\alpha)^\top,\end{array}\right.$	$\left.\begin{array}{ll}18, & 0 \leq \alpha < 0.3\\ 15+10\alpha, & 0.3 \leq \alpha \leq 1\end{array}\right\}$
$\mathbf{x}^3 = (0,1)^\top$	$(12,0)^\top$	34	$(3,9)^\top$	25	$\left\{\begin{array}{l}(3,3)^\top,\\ (3,12\alpha-3)^\top,\end{array}\right.$	$\left.\begin{array}{ll}19, & 0 \leq \alpha < 0.5\\ 13+12\alpha, & 0.5 \leq \alpha \leq 1\end{array}\right\}$

According to Figure 2(a), the leader's optimal α–pessimistic decision is $\mathbf{x}^3$ for $0 \leq \alpha \leq 0.4$ and $\mathbf{x}^2$ for $0.4 \leq \alpha \leq 1$. This figure also shows that for $\alpha = 1$, both decisions result in the same objective function value, which corresponds to an optimal pessimistic solution. In

Figure 2(b) the leader's optimal objective function value in optimistic, pessimistic and α–pessimistic cases is depicted; furthermore, we provide the value of $\alpha f_p^* + (1-\alpha) f_0^*$, which is an upper bound for f_α^* according to Corollary 2.

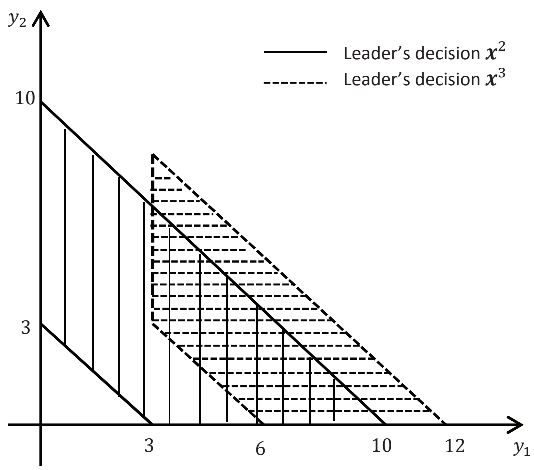


Figure 1: Follower's feasible region for leader's decisions $\mathbf{x}^2$ and $\mathbf{x}^3$. Note that $\mathbf{x}^1 = (0,0)^\top$ and $\mathbf{w}(\mathbf{x}^1) = \mathbf{y}^p(\mathbf{x}^1) = \mathbf{y}^\alpha(\mathbf{x}^1) = (0,0)^\top$.

Figure 2(c) illustrates the value of $\delta_{0,\alpha}$, i.e., the "loss" of a conservative decision-maker, who implements optimal 0-pessimistic solution $\bar{x}^0$ (i.e., a solution of the max-min problem, where the follower's objective function is completely ignored), while the follower is, in fact, α-pessimistic. It is intuitive that for smaller values of α this "loss" is reasonably small. However, it is interesting to observe that for values of α close to 1, the "loss" of the leader's is also rather small, which illustrates the fact that the value of $\delta_{\alpha_1,\alpha_2}$ does not necessarily increase if the difference $\alpha_2 - \alpha_1$ increases. In Figure 2(c) we also depict the value of $f_\alpha^* - f_0^*$, which is an upper bound for $\delta_{0,\alpha}$ according to Corollary 4. For smaller values of α the quality of this upper bound is rather good; however, as α increases its quality deteriorates. Both of these observations are rather intuitive as f_α^* is a non-decreasing function (see Proposition 6), while by its definition $\delta_{\alpha_1,\alpha_2}$ should be relatively small for sufficiently small values of $\alpha_2 - \alpha_1$ (recall that $\delta_{\alpha,\alpha} = 0$).

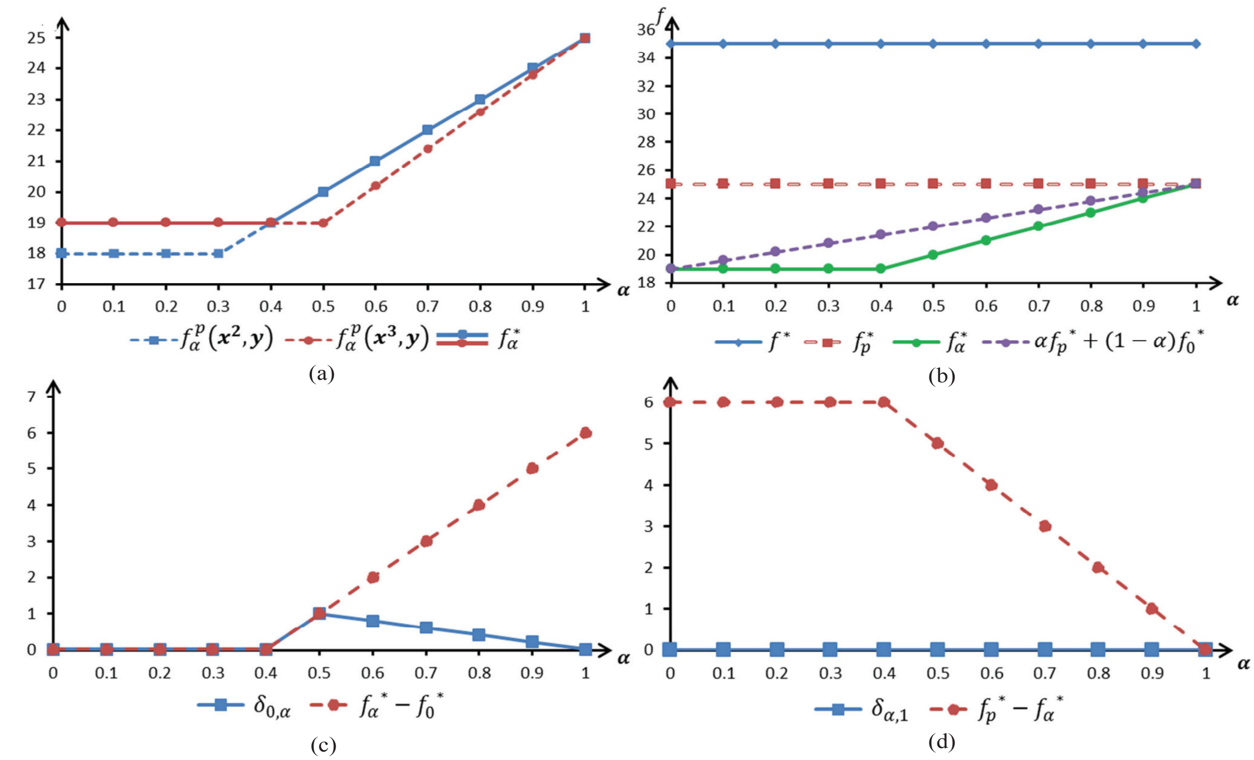


Figure 2: Illustration of structural results for a **BMIP** example given by (2.13).

Figure 2(d) is similar in spirit to Figure 2(c). Specifically, we first depict the value of $\delta_{\alpha,1} = f_1^* - f_1^p(\bar{x}^\alpha) = f_p^* - f^p(\bar{x}^\alpha)$, i.e., the "loss" of the conservative decision-maker, who implements optimal α-pessimistic solution $\bar{x}^\alpha$, while the follower is, in fact, simply pessimistic. Figure 2(d) demonstrates that in the considered example, the decision-maker does not lose anything by being conservative as $\delta_{\alpha,1} = 0$ for all values of α. Clearly, this is not necessarily the case in general. In Figure 2(d) we also provide the value of $f_p^* - f_\alpha^*$, which is an upper bound for $\delta_{\alpha,1}$ according to Corollary 4. The quality of this upper bound is relatively poor for smaller values of α, but improves as α gets closer to 1. Such behavior is intuitive if one recalls the definition of $\delta_{\alpha,1}$ in (2) and observes that the value of $1 - \alpha$ decreases as α increases. Some additional numerical illustrations of the developed theoretical results are provided in Section 2.5, where we consider an application example of **BMIP**.

Concluding this section, we note that our approach has connections to ϵ-regularized version of general bilevel problems, see, e.g., [75], where the follower's response is assumed to return an objective function value that is within ϵ from optimal. However, such studies typically consider more general functional forms of the upper- and lower-level optimization problems (not linear as in our case) and they primarily derive stability and existence results. Thus, the motivation behind studying such classes of problems is different from ours.

2.4 STRONG-α-WEAK RESPONSE TO THE LEADER'S DECISION

The optimistic and pessimistic (also often referred to as strong and weak, see [31]) formulations of BMIP model two extreme cases of possible relationships between the leader and the follower. As discussed in detail in Section 2.1, the leader assumes that the follower is fully cooperative in the optimistic formulation; whereas in the pessimistic formulation, the leader expects an adversarial response from the follower.

To generalize these two approaches, Aboussoror and Loridan [1] define the term strong-weak Stackelberg problem to model partial cooperation between the leader and the follower. They integrate the optimistic and pessimistic formulations through a weighted summation of the leader's objective functions in the optimistic and pessimistic cases. The coefficients in this summation are set by the leader and can be interpreted as the probabilities of cooperation or non-cooperation of the follower, respectively. In a similar manner, Cao and Leung [31] describe a BLP with partial cooperation for the linear version of the strong-weak Stackelberg problem. They reformulate the bilevel model into a single-level model using penalty coefficients, and present a numerical example, where the follower's optimal approach is to cooperate partially. In other words, in some cases the follower could achieve the optimization of his interests when he partially cooperates with the leader [31]. Zheng et al. [119] show that the leader's optimal value function is piece-wise linear and monotone in the weight coefficient measuring the follower's level of cooperation (see our related discussion of Propositions 10 and 11 below). They also present an exact penalty method to solve the strong-weak BLP for every fixed weight.

In this section, we generalize the strong-weak BLP by considering an α-pessimistic follower considered in Section 2.3. Similar to the strong-weak approach described in the previous paragraph, we also use a weight coefficient to integrate those two extremes. Specifically, given $\alpha \in [0,1]$ and cooperation coefficient $\gamma \in [0,1]$, the leader solves the following optimization problem:

$$[(\gamma,\alpha)\text{-}\mathbf{BMIP}] \quad \max_{x\in\mathbb{X}} \left\{ c^\top x + (1-\gamma) \min_{y\in H_\alpha(x)} d_1^\top y + \gamma \max_{y\in H(x)} d_1^\top y \right\}, \tag{2.14}$$

where at one extreme the follower might fully cooperate with the leader, see the last term in (2.14), but at the other extreme, he might give up $1-\alpha$ portion of his optimal objective function value in order to inflict more damage to the leader, see the second term in (2.14).

It is important to note that (γ,α)-**BMIP** contains as its special cases the max-min problem (2.8) as well as the pessimistic and optimistic models given by (2.1) and (2.3), respectively. Formally, if $\alpha = 1$ then (γ,α)-**BMIP** reduces to the strong-weak formulation from [31, 119], where $(0,1)$-**BMIP** corresponds to the pessimistic **BMIP**, while $(1,\alpha)$-**BMIP** reduces to the optimistic **BMIP** for any $\alpha \in [0,1]$. On the other hand, if $\alpha = 0$, then the second term in the objective function of (γ,α)-**BMIP**, namely, the one that optimizes over $y \in H_\alpha(x)$, corresponds to the solution of the max-min problem (2.8). Thus, the proposed approach, further referred to as the strong-α-weak problem, can be viewed as a natural generalization of the strong-weak approach, where we consider more general types of adversarial followers by using $\alpha \in [0,1]$.

Let $\bar{x}_\gamma^\alpha$ be the leader's optimal solution to (γ,α)-**BMIP**. Recall from Section 2.3 that x^* and $\bar{x}^\alpha$ are the leader's optimal solutions in the optimistic and α-pessimistic formulations, respectively. Thus, $\bar{x}_1^\alpha = x^*$ and $\bar{x}_0^\alpha = \bar{x}^\alpha$. Furthermore, denote by $f^*_{\gamma,\alpha}$ the optimal objective function value of (γ,α)-**BMIP**, that is $f^*_{\gamma,\alpha} = f^{\gamma,\alpha}(\bar{x}_\gamma^\alpha)$. Next, we analyze basic properties of $f^*_{\gamma,\alpha}$.

Proposition 10. *For any $\alpha \in [0,1]$, $f^*_{\gamma,\alpha}$ is non-decreasing in $\gamma \in [0,1]$.*

Remark 3. It is rather straightforward to show that for any γ_1 and γ_2, such that $1 \geq \gamma_1 \geq \gamma_2 \geq 0$, we have

$$f^* \geq f^*_{\gamma_1,1} \geq f^*_{\gamma_2,1} \geq f^*_p.$$

Therefore, if there exists a leader's optimal solution $\widetilde{x}$ that is optimal for both optimistic and pessimistic cases of BMIP and ensures that $f^* = f(\widetilde{x}) = f^p(\widetilde{x}) = f^*_p$, then this solution is obtained by solving (γ,α)-**BMIP** for any $\gamma \in [0,1]$ and $\alpha = 1$. Thus, $f^* = f^*_{\gamma,1} = f^*_p$ for any $\gamma \in [0,1]$. On the other hand, if the decision-maker solves the optimistic and pessimistic cases of **BMIP** separately, then it is not guaranteed that such solution is obtained. In other words, the equality $f^* = f^*_p$ can be checked by solving the optimistic and pessimistic cases of BMIP separately. However, the corresponding leader's solutions x^* and $\bar{x}^1$ are not necessarily optimal for $\mathbf{BMIP}^{\text{pes}}$and $\mathbf{BMIP}^{\text{opt}}$, respectively. This observation can be viewed as another advantage of the strong-weak approach, in particular, when the decision-maker is not aware if the follower is collaborative or adversarial.

Proposition 11. *For any $\alpha \in [0,1]$, $f^*_{\gamma,\alpha}$ is convex in $\gamma \in [0,1]$.*

Proof. Let $0 \le \gamma_1 \le \gamma_2 \le 1$, and $\gamma = \theta\gamma_1 + (1-\theta)\gamma_2$ for $\theta \in [0,1]$. Then:

$$
\begin{aligned}
f^*_{\gamma,\alpha} &= c^\top \bar{x}^\alpha_\gamma + (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \\
&= \theta \left(c^\top \bar{x}^\alpha_\gamma + (1-\gamma_1) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + \gamma_1 d_1^\top w(\bar{x}^\alpha_\gamma) \right) + \\
&\qquad\qquad (1-\theta) \left(c^\top \bar{x}^\alpha_\gamma + (1-\gamma_2) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + \gamma_2 d_1^\top w(\bar{x}^\alpha_\gamma) \right) \\
&\le \theta \left(c^\top \bar{x}^\alpha_{\gamma_1} + (1-\gamma_1) d_1^\top y^\alpha(\bar{x}^\alpha_{\gamma_1}) + \gamma_1 d_1^\top w(\bar{x}^\alpha_{\gamma_1}) \right) + \\
&\qquad\qquad (1-\theta) \left(c^\top \bar{x}^\alpha_{\gamma_2} + (1-\gamma_2) d_1^\top y^\alpha(\bar{x}^\alpha_{\gamma_2}) + \gamma_2 d_1^\top w(\bar{x}^\alpha_{\gamma_2}) \right) \\
&\le \theta f^*_{\gamma_1,\alpha} + (1-\theta) f^*_{\gamma_2,\alpha},
\end{aligned}
$$

which implies the required result. ∎

If $\alpha = 1$, then, as mentioned earlier, the proposed strong-α-weak model given by (γ,α)-**BMIP** reduces to the strong-weak model from the literature, and the structural results derived in Propositions 10 and 11 are equivalent to those shown in [119]. However, our derivations demonstrate that these results, namely, the non-decreasing and convexity properties of $f^*_{\gamma,\alpha}$, also hold for the case when the follower is α-pessimistic for any $\alpha \in [0,1]$. Furthermore:

Proposition 12. *For any $\gamma \in [0,1]$, $f^*_{\gamma,\alpha}$ is convex in $\alpha \in [0,1]$.*

Proof. Let $0 \le \alpha_1 \le \alpha_2 \le 1$, and $\alpha = \theta\alpha_1 + (1-\theta)\alpha_2$ for $\theta \in [0,1]$. Let $\widetilde{y} = \theta y^{\alpha_1}(\bar{x}^\alpha_\gamma) + (1-\theta)y^{\alpha_2}(\bar{x}^\alpha_\gamma)$. As in the proof of Proposition 7, we can show that $\widetilde{y} \in H_\alpha(\bar{x}^\alpha_\gamma)$ and $d_1^\top \widetilde{y} \ge d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)$. Then,

$$\begin{aligned} f^*_{\gamma,\alpha} =& c^\top \bar{x}^\alpha_\gamma + (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \le c^\top \bar{x}^\alpha_\gamma + (1-\gamma) d_1^\top \widetilde{y} + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \\ =& \, \theta \left(c^\top \bar{x}^\alpha_\gamma + (1-\gamma) d_1^\top y^{\alpha_1}(\bar{x}^\alpha_\gamma) + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \right) + \\ & \qquad\qquad (1-\theta) \left(c^\top \bar{x}^\alpha_\gamma + (1-\gamma) d_1^\top y^{\alpha_2}(\bar{x}^\alpha_\gamma) + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \right) \\ \le& \, \theta f^*_{\gamma,\alpha_1} + (1-\theta) f^*_{\gamma,\alpha_2}, \end{aligned}$$

which concludes the proof. ∎

One natural question that arises when comparing the strong-α-weak model against either optimistic or pessimistic cases of **BMIP** is that how much the leader "loses" in terms of the obtained objective function value if the follower is, in fact, either optimistic or α-pessimistic, respectively. Next, we provide bounds on these differences. First, we derive an upper bound for the difference between f^*, i.e., the optimal objective value of the leader in the optimistic formulation, and $f(\bar{x}^\alpha_\gamma)$, i.e., the objective value of the leader if she implements $\bar{x}^\alpha_\gamma$ in the optimistic case.

Proposition 13. *For any $\gamma \in [0,1]$ and $\alpha \in [0,1]$, $f^* - f(\bar{x}^\alpha_\gamma) \le (1-\gamma)\left(d_1^\top w(x^*) - d_1^\top y^\alpha(x^*)\right)$*

Proof.

$$\begin{aligned} f(\bar{x}^\alpha_\gamma) &= c^\top \bar{x}^\alpha_\gamma + d_1^\top w(\bar{x}^\alpha_\gamma) \\ &= c^\top \bar{x}^\alpha_\gamma + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) + (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + (1-\gamma) d_1^\top w(\bar{x}^\alpha_\gamma) - (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) \\ &\ge c^\top x^* + \gamma d_1^\top w(x^*) + (1-\gamma) d_1^\top y^\alpha(x^*) + (1-\gamma) d_1^\top w(\bar{x}^\alpha_\gamma) - (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) \\ &\ge c^\top x^* + \gamma d_1^\top w(x^*) + (1-\gamma) d_1^\top y^\alpha(x^*) \\ &= c^\top x^* + d_1^\top w(x^*) - (1-\gamma)\left(d_1^\top w(x^*) - d_1^\top y^\alpha(x^*)\right) \\ &= f^* - (1-\gamma)\left(d_1^\top w(x^*) - d_1^\top y^\alpha(x^*)\right), \end{aligned}$$

where the last inequality follows from the fact that $d_1^\top w(\bar{x}^\alpha_\gamma) \ge d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)$. ∎

Moreover, our next result shows that if c and d_1 are nonnegative, then $\bar{x}^\alpha_\gamma$ provides a γ-approximate solution to the optimistic **BMIP**. In other words, the decision-maker has some guaranteed quality of the obtained solution if the follower turns out to be collaborative.

Corollary 5. *If $c \in \mathbb{R}^{n_1}_+$ and $d_1 \in \mathbb{R}^{n_2}_+$, then $f(\bar{x}^\alpha_\gamma) \geq \gamma f^*$.*

Proof.

$$\begin{aligned} f(\bar{x}^\alpha_\gamma) \geq & f^* - (1-\gamma)\left(d_1^\top w(x^*) - d_1^\top y^\alpha(x^*)\right) \geq \ f^* + (1-\gamma)\left(-d_1^\top w(x^*)\right) \\ & \geq f^* + (1-\gamma)\left(-d_1^\top w(x^*) - c^\top x^*\right) = f^* + (1-\gamma)(-f^*) = \gamma f^*. \end{aligned}$$

■

Next, we consider an adversarial follower. In particular, we derive an upper bound for the difference between f^*_α, i.e., the optimal objective function value of the leader in the α-pessimistic formulation, and $f^p_\alpha(\bar{x}^\alpha_\gamma)$, i.e., the objective function value of the leader if she implements $\bar{x}^\alpha_\gamma$ in the α-pessimistic case.

Proposition 14. *For $0 \leq \alpha, \gamma \leq 1$ we have that $f^*_\alpha - f^p_\alpha(\bar{x}^\alpha_\gamma) \leq \gamma\left(d_1^\top w(\bar{x}^\alpha_\gamma) - d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)\right)$.*

Proof.

$$\begin{aligned} f^p_\alpha(\bar{x}^\alpha_\gamma) &= c^\top \bar{x}^\alpha_\gamma + d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) \\ &= c^\top \bar{x}^\alpha_\gamma + \gamma d_1^\top w(\bar{x}^\alpha_\gamma) + (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) + \gamma d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) - \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \\ &\geq c^\top \bar{x}^\alpha + \gamma d_1^\top w(\bar{x}^\alpha) + (1-\gamma) d_1^\top y^\alpha(\bar{x}^\alpha) + \gamma d_1^\top y(\bar{x}^\alpha_\gamma) - \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \\ &= c^\top \bar{x}^\alpha + d_1^\top y(\bar{x}^\alpha) + \gamma d_1^\top w(\bar{x}^\alpha) - \gamma d_1^\top y^\alpha(\bar{x}^\alpha) + \gamma d_1^\top y^\alpha(\bar{x}^\alpha_\gamma) - \gamma d_1^\top w(\bar{x}^\alpha_\gamma) \\ &\geq f^*_\alpha - \gamma\left(d_1^\top w(\bar{x}^\alpha_\gamma) - d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)\right), \end{aligned}$$

where the last inequality follows from the fact that $d_1^\top w(\bar{x}^\alpha) \geq d_1^\top y^\alpha(\bar{x}^\alpha)$. ■

Note that finding $\bar{x}^\alpha_\gamma$ is an NP-hard problem. However, given $\bar{x}^\alpha_\gamma$ the values of $d_1^\top w(\bar{x}^\alpha_\gamma)$ and $d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)$ can be computed by solving linear programming problems. Therefore, the upper bound for $f^*_\alpha - f^p_\alpha(\bar{x}^\alpha_\gamma)$ given by Proposition 14 can be obtained in polynomial time after finding $\bar{x}^\alpha_\gamma$.

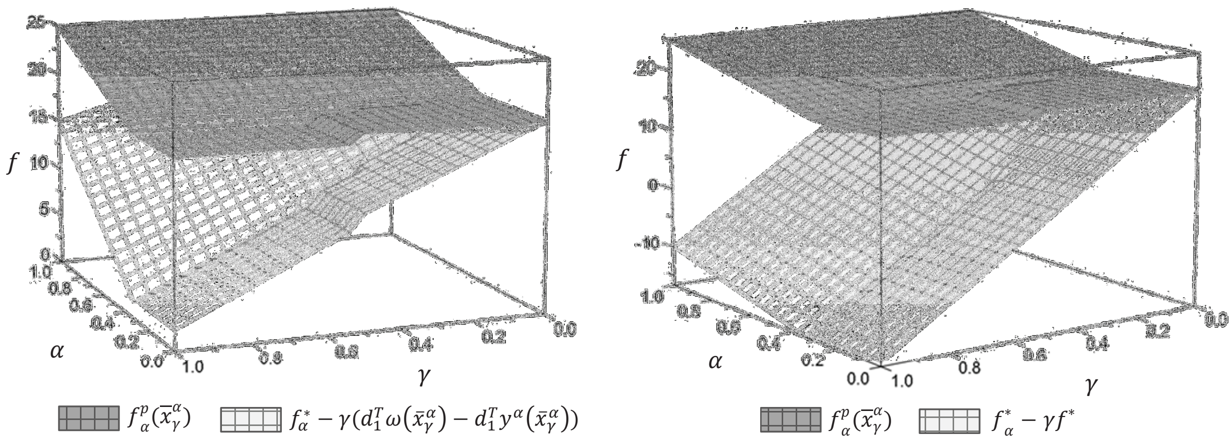
Corollary 6. *If $c \in \mathbb{R}^{n_1}_+$ and $d_1 \in \mathbb{R}^{n_2}_+$, then $f^p_\alpha(\bar{x}^\alpha_\gamma) \geq f^*_\alpha - \gamma f(\bar{x}^\alpha_\gamma) \geq f^*_\alpha - \gamma f^*$.*

Proof. It follows from Proposition 14 that

$$\begin{aligned} f^p_\alpha(\bar{x}^\alpha_\gamma) &\geq f^*_\alpha - \gamma\left(d_1^\top w(\bar{x}^\alpha_\gamma) - d_1^\top y^\alpha(\bar{x}^\alpha_\gamma)\right) \geq f^*_\alpha + \gamma\left(-d_1^\top w(\bar{x}^\alpha_\gamma)\right) \\ &\geq f^*_\alpha + \gamma\left(-d_1^\top w(\bar{x}^\alpha_\gamma) - c^\top \bar{x}^\alpha_\gamma\right) = f^*_\alpha - \gamma f(\bar{x}^\alpha_\gamma) \geq f^*_\alpha - \gamma f^*, \end{aligned}$$

which concludes the proof. ■

For the example given by (2.13), Figure 3 illustrates the bounds obtained in Proposition 14 and Corollary 6. Clearly, the quality of the former bound is better, which is not surprising given the provided derivations. On the other hand, it is also worth mentioning that the quality of the bounds improves as α and γ approach one and zero, respectively. This observation is rather intuitive as (0,1)-**BMIP** corresponds to the pessimistic case of **BMIP**.



(a) (b)

Figure 3: Illustration of Proposition 14 and Corollary 6 for a **BMIP** example given by (2.13).

Assume that there exist a positive lower bound L^*_α for f^*_α and a finite upper bound U^* for f^*, that is,

$$0 < L^*_\alpha \leq f^*_\alpha \leq f^* \leq U^* < +\infty. \tag{2.15}$$

Then we have the following result, which is similar in spirit to Corollary 5:

Corollary 7. *If $c \in \mathbb{R}^{n_1}_+$, $d_1 \in \mathbb{R}^{n_2}_+$ and $f^*_\alpha > 0$, then for a given $\bar{\gamma} \in [0,1]$, define $\gamma = (1-\bar{\gamma})\frac{L^*_\alpha}{U^*}$. Then $f^p_\alpha(\bar{x}^\alpha_\gamma) \geq \bar{\gamma} f^*_\alpha$ and $f(\bar{x}^\alpha_\gamma) \geq \gamma f^*$.*

Proof. By using Corollary 6, we have

$$f^p_\alpha(\bar{x}^\alpha_\gamma) \geq f^*_\alpha - \gamma f^* = f^*_\alpha - (1-\bar{\gamma}) \cdot \frac{L^*_\alpha}{U^*} \cdot f^* \geq f^*_\alpha - (1-\bar{\gamma}) \cdot L^*_\alpha \geq f^*_\alpha - (1-\bar{\gamma}) \cdot f^*_\alpha = \bar{\gamma} f^*_\alpha,$$

where we use (2.15) in the obtained inequalities. ■

The above results provide the leader with some estimates of her loses in cases when the follower is either optimistic or α-pessimistic. In particular, under some assumptions $\bar{x}_\gamma^\alpha$ provides simultaneously a γ-approximate solution to the optimistic **BMIP** and $\bar{\gamma}$-approximate solution to the α-pessimistic **BMIP**. Note that the relationship between γ and $\bar{\gamma}$ through some lower and upper bounds for f_α^* and f^* is rather intuitive given our earlier observations in Remarks 1 and 2.

2.5 NUMERICAL ILLUSTRATIONS

In this section, we provide additional illustrations of the proposed modeling approach using a class of defender-attacker problems. In our numerical experiments we solve single-level reformulations of our models using CPLEX 12.4 [67].

2.5.1 Single-level Reformulations

We reformulate $\mathbf{BMIP}^{\text{opt}}$, $\mathbf{BMIP}^{\text{pes}}$, α-$\mathbf{BMIP}^{\text{pes}}$and (γ, α)-**BMIP** as single-level mixed-integer programs with constraints that enforce primal feasibility, dual feasibility, and complementary slackness for the follower's linear program. It is a standard approach in the bilevel optimization literature, which can be applied as long as the follower's problem is an LP, see, e.g., [9] for more detailed discussion in the case of optimistic bilevel programs. The fact that both α-$\mathbf{BMIP}^{\text{pes}}$ and (γ, α)-**BMIP** admit single-level MIP reformulations can be viewed as another advantage of the proposed modeling approach.

For completeness of the discussion we first present the standard single-level formulation for $\mathbf{BMIP}^{\text{opt}}$, see, e.g., [9]:

$$
\begin{aligned}
[\mathbf{BMIP}^{\text{opt}}] : \max \quad & c^\top x + d_1^\top y && && (2.16a)\\
\text{s.t. } & x \in \mathbb{X} && && (2.16b)\\
& By \leq h - Ax && (\lambda) && (2.16c)\\
& By \geq h - Ax - M_\lambda(e - u_\lambda) && && (2.16d)\\
& \lambda \leq M_\lambda u_\lambda && && (2.16e)\\
& B^\top \lambda \geq d_2 && (y) && (2.16f)\\
& B^\top \lambda \leq d_2 + M_y(e - u_y) && && (2.16g)\\
& y \leq M_y u_y && && (2.16h)\\
& u_\lambda \in \{0,1\}^{m_2}, u_y \in \{0,1\}^{n_2},\ y, \lambda \geq 0, && && (2.16i)
\end{aligned}
$$

where e is the vector of all ones of appropriate dimensions, i.e., $e = (1, \ldots, 1)^\top$, while M_λ and M_y are sufficiently large positive constants. Constraints (2.16c)-(2.16i) ensures that $y \in H(x)$ by enforcing primal feasibility, dual feasibility, and complementary slackness conditions for the follower's LP given the leader's decision x. In particular, λ is the set of dual variables corresponding to constraints (2.16c) in the follower's LP, while 0–1 variables u_λ and u_y are used to linearize the complementary slackness conditions.

Next, we present the single-level reformulation for (γ, α)-**BMIP**:

$$
\begin{aligned}
[(\gamma,\alpha)\text{-}\mathbf{BMIP}] : \max\ & c^\top x + \gamma d_1^\top y + (1-\gamma) d_1^\top y' && && \text{(2.17a)}\\
\text{s.t. } & (2.16b) - (2.16i) && && \\
& By' \le h - Ax && (\mu) && \text{(2.17b)}\\
& By' \ge h - Ax - M_\mu(e - u_\mu) && && \text{(2.17c)}\\
& \mu \le M_\mu u_\mu && && \text{(2.17d)}\\
& d_2^\top y' \ge \alpha d_2^\top y + (1-\alpha)L && (\zeta) && \text{(2.17e)}\\
& d_2^\top y' \le \alpha d_2^\top y + (1-\alpha)L + M_\zeta(1 - u_\zeta), && && \text{(2.17f)}\\
& \zeta \le M_\zeta u_\zeta, && && \text{(2.17g)}\\
& d_2\zeta - B^\top \mu \le d_1, && (y') && \text{(2.17h)}\\
& d_2\zeta - B^\top \mu \ge d_1 - M_{y'}(e - u_{y'}), && && \text{(2.17i)}\\
& y' \le M_{y'} u_{y'}, && && \text{(2.17j)}\\
& u_\mu \in \{0,1\}^{m_2}, u_{y'} \in \{0,1\}^{n_2},\ u_\zeta \in \{0,1\},\ y', \mu, \zeta \ge 0, && && \text{(2.17k)}
\end{aligned}
$$

where M_μ, M_ζ, $M_{y'}$ are sufficiently large positive constants. Constraints (2.17b)-(2.17k) impose that the follower chooses a solution $y' \in H_\alpha(x)$ that provides the minimum $d_1^\top y'$ for the leader. The main ideas behind formulation (2.17) is similar to those used in deriving (2.16). In particular, y and y' are variables representing the optimistic and the α-pessimistic responses of the follower, respectively. Also, ζ and μ are the dual variables corresponding to constraints in $H_\alpha(x)$, see (2.6), given the leader's decision x.

If $\gamma = 0$ and $\alpha = 1$ in formulation (2.17), then we obtain a single-level reformulation for the pessimistic BMIP. Furthermore, if $\gamma > 0$ and $\alpha = 1$, then we obtain a single-level reformulation for the strong-weak bilevel linear program [31]. Note that Zeng [116] provides similar reformulations for the strong-weak BMIP. Thus, model (2.17) generalizes the formulations presented in Zeng [116] by considering follower's α-suboptimal response to the leader, i.e., the strong-α-weak approach considered in Section 2.4.

2.5.2 Defender-Attacker Problem (DAP)

There are a number of defender-attacker models proposed in the related literature, see some examples in [27] and the references therein. In this section we consider a class of such models, where the defender (leader) runs a set of facilities J. Facility $j \in J$ has a certain value (e.g., capacity) given by c_j and can be fully protected by spending k_j units of the defender's resource. The total defense budget is K units. The attacker (follower) can destroy $y_j \in [0,1]$ portion of the facility j by spending $b_j y_j$ units. The attacker's goal is to minimize the leader's total value after the attack (i.e., maximize damage) subject to a budget constraint of B units. If y_j portion of the facility value is destroyed, then the defender has to spend $r_j y_j$ units to recover its full value. The defender's objective is to minimize the total recovery cost. We formulate the considered class of pessimistic DAPs as:

$$[\text{pes-}\mathbf{DAP}] \quad \min_{x\in\mathbb{X}} \max_{y\in H(x)} \sum_{j\in J} r_j y_j$$
$$\text{subject to } H(x) = \operatorname{argmax}\left\{\sum_{j\in J} c_j y_j : y \in \mathbb{Y}, y_j \leq 1 - x_j,\ j \in J\right\},$$

where $\mathbb{X} \subseteq \{x \in \{0,1\}^{|J|} \ :\ \sum_{j\in J} k_j x_j \leq K\}$ and $\mathbb{Y} = \{y \in [0,1]^{|J|} \ :\ \sum_{j\in J} b_j y_j \leq B\}$. The leader's decision variable, x_j, is equal to 1 iff facility j is protected and 0, otherwise. The follower's decision variable, $y_j \in [0,1]$, represents the destroyed portion of facility j. Given $\alpha \in [0,1]$ and $\gamma \in [0,1]$, (γ,α)–**DAP** can be formulated as:

$$[(\gamma,\alpha)\text{-}\mathbf{DAP}] \quad \min_{x\in\mathbb{X}} \left\{(1-\gamma)\max_{y\in H_\alpha(x)} \sum_{j\in J} r_j y_j + \gamma \min_{y\in H(x)} \sum_{j\in J} r_j y_j\right\},$$

where the suboptimal reaction set of the attacker is defined as:

$$H_\alpha(x) = \{y' \in \mathbb{Y} :\ \sum_{j\in J} c_j y'_j \geq \alpha \sum_{j\in J} c_j y_j,\ y \in H(x),\ y'_j \leq 1 - x_j,\ j \in J\}.$$

Next, we illustrate some of the structural properties derived in Sections 2.3 and 2.4. We consider a DAP instance with 10 facilities. Parameters of the instance include the recovery cost vector $\mathbf{r} = [19\ 21\ 25\ 29\ 31\ 35\ 36\ 40\ 43\ 58]^\top$, the capacity vector $\mathbf{c} = [10\ 10\ 10\ 9\ 8\ 7\ 6\ 5\ 4\ 3]^\top$, facility protection cost $k_j = 1$ and destruction cost $b_j = 1$ for all $j = 1,\ldots,10$, the total defense budget $K = 2$ and the attacker's budget is $B = 1$.

Furthermore, the defender has two additional logical constraints of the form: $x_1+x_2+x_3 \leq 1$ and $x_9 \leq x_1$, which are incorporated into the constraint set defining $\mathbb{X}$.

Recall that our example (2.13) is a "max-max" **BMIP**. On the other hand, the considered class of DAPs involves minimization of the leader's objective function. As briefly discussed in Section 2.3, some simple adjustments are necessary when we apply the results from Sections 2.3 and 2.4 to the considered class of DAPs. For example, f^*_α is non-increasing with respect to α instead of non-decreasing as stated in Proposition 6. Alternatively, one could obtain maximization version of **DAP** by simply changing the signs of r_j's, and thus, directly apply the results of Sections 2.3 and 2.4.

Figure 4 illustrates various structural properties established in Section 2.3. In particular, it is interesting to observe in Figure 4(a) that the value of Δ_α decreases as α increases. This result is rather intuitive if one recalls that $H_{\alpha_1}(x) \subseteq H_{\alpha_2}(x)$ for $\alpha_1 \geq \alpha_2$, i.e., the follower has more flexibility in making the decision less favorable for the leader for smaller values of α. Figure 4(b) depicts Δ_α along with its upper and lower bounds derived in Proposition 8 and Corollary 3. Figures 4(c) and 4(d) are analogous to Figures 2(c) and 2(d), respectively.

Figure 5 illustrates Propositions 13 and 14 established in Section 2.4. The obtained graphics match the intuition behind (γ, α)-**BMIP** model and the derived results. For example, in Figure 5(a) the depicted functions coincide for $\gamma = 1$, which, in fact, should be expected as $(1, \alpha)$-**BMIP** corresponds to optimistic **BMIP** for any $\alpha \in [0, 1]$. Similarly, in Figure 5(b) the depicted functions also coincide for $\gamma = 0$ as $(0, \alpha)$-**BMIP** corresponds to α-pessimistic **BMIP**. Finally, the quality of the bounds from Propositions 13 and 14 is better for larger and smaller values of γ in Figures 5(a) and 5(b), respectively. These observations are natural if one recalls the motivation behind (γ, α)-**BMIP** model, in particular, the fact that the objective function of (γ, α)-**BMIP** is a convex combination of the follower's optimistic and α-pessimistic responses to the leader's decision.

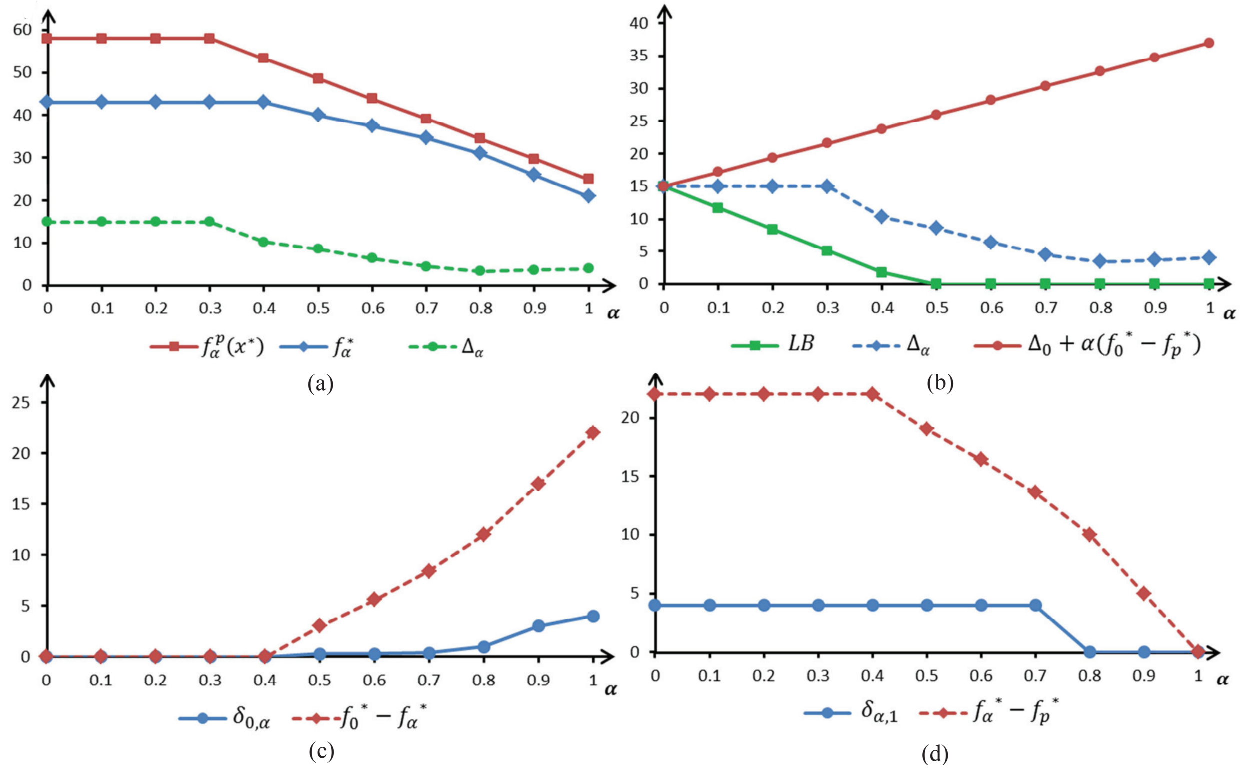


Figure 4: Illustration of structural results with a **DAP** instance from Section 2.5.2. Note that the leader's problem involves minimization, which requires some minor adjustments in the corresponding statements of Section 2.3, see related discussion in Sections 2.3 and 2.5.2. The term "LB" in Figure 4(b) stands for the lower bound of Δ_α in Proposition 8. Figures 4(c) and 4(d) are analogous to Figures 2(c) and 2(d), respectively.

2.6 CONCLUDING REMARKS

In this chapter we study relationships between optimistic and pessimistic BLPs and BMIPs, where the follower's optimization problem is a linear program. First, we focus on theoretical computational complexity issues for BLPs. Perhaps, the most interesting complexity result obtained is the fact that even if an optimal optimistic (or pessimistic) solution of BLP is known, then the problem of finding an optimal pessimistic (or optimistic) solution for the same BLP remains an NP-hard problem. Second, we propose a generalization of

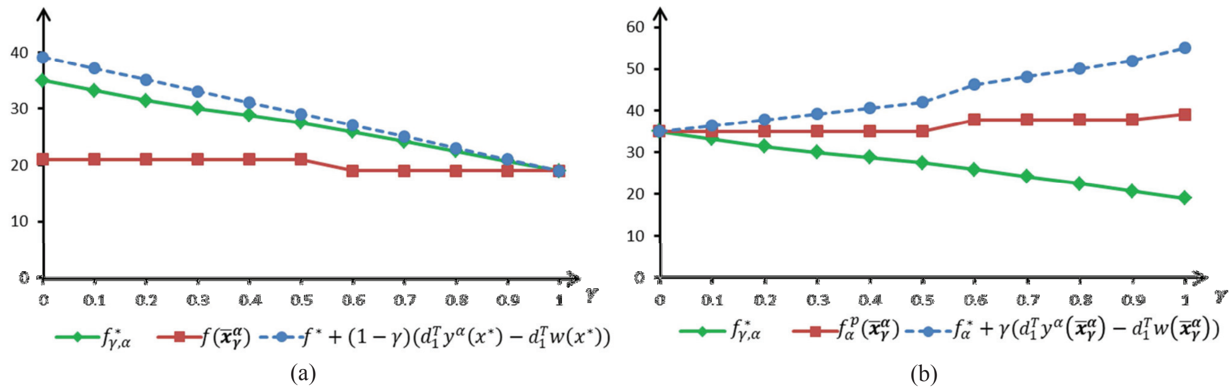


Figure 5: Illustration of Propositions 13 and 14 with a **DAP** instance from Section 2.5.2 for $\alpha = 0.7$. Note that the leader's problem involves minimization.

pessimistic bilevel linear problems, referred to as α-pessimistic BMIPs, where the follower might willingly give up a portion of his optimal objective function value, and thus select a suboptimal solution in order to inflict more damage to the leader. It is important to note that our techniques allow the decision-maker to consider more general types of adversarial followers. In particular, α-pessimistic BMIPs naturally encompasses as their special classes both pessimistic BMIPs and max-min (or min-max) problems. Furthermore, we incorporate the proposed approach into a class of strong-weak models that capture settings, where the leader is not certain if the follower is either collaborative or adversarial, and thus attempts to make a robust decision by taking into account the follower's response in both situations. Finally, we study structural properties of the proposed mathematical models and illustrate the obtained results using insightful numerical examples.

3.0 ON BILEVEL OPTIMIZATION WITH INEXACT FOLLOWER

3.1 INTRODUCTION

Motivation. In bilevel optimization, a *leader* solves an *upper-level* formulation whose objective function depends on a set of *lower-level* decisions, which in turn are made by a *follower* in reaction to the leader's (upper-level) decisions ([12, 38]).In this framework, the upper-level decisions might affect the lower-level objective function and/or feasible region, and are considered as an input by the follower, who is traditionally assumed to react optimally to them. The outlined setting suggests that, while the leader is able to act strategically by anticipating the follower's (optimal) reaction, the follower's role is rather reactionary. For this reason, bilevel optimization is typically used to, for example, model Stackelberg games ([50]), and has been also applied in many areas to model the interaction between rational agents that make decisions sequentially.

A key assumption in bilevel optimization is that both the leader and follower have the computational means to solve the upper- and lower-level formulations optimally, respectively. However, in many important application areas, one has that either: (i) there is no known efficient method to solve the lower-level formulation to optimality (for a given set of upper-level decisions); or (ii) the follower either is not sufficiently sophisticated or does not have the computational resources necessary to find an optimal solution to the lower-level problem in a timely manner. In both cases, the follower typically resorts to using computationally-tractable heuristic/approximate algorithms.

In particular, for a given leader's decision the lower-level optimization problem may correspond to a medium- or large-sized instance of an NP-hard problem: while exact algorithms may be available, they often take prohibitively large computing time to produce optimal solutions. A concrete and, perhaps, the simplest example of such a lower-level formulation is the linear *0–1 knapsack problem*, which is NP-hard ([54]). In the bilevel optimization literature, problems that involve knapsack-like constraints at the lower level are known as bilevel knapsack problems (see [18, 26, 32, 86]). Exact algorithms for single- and multi-dimensional 0–1 knapsack problems aim at intelligent enumeration of feasible solutions, e.g., based on branch-and-bound schemes (see [64, 76]), dynamic programming (see [64, 105]). While a number of such algorithms are specially tailored to solve large-scale instances (see, e.g., [11, 47, 73, 77]), in the worst case it takes them an exponential running time to find an optimal solution.

In general, when faced with such "hard" optimization models, a common approach in many practical settings is to resort to either heuristic or approximation algorithms that find good solutions in reasonable time. For example, many such algorithms have been proposed to find approximate solutions for the linear 0–1 knapsack problem, including a simple greedy-based 1/2-approximation algorithm (see, e.g., [73]) and more complex fully polynomial-time approximation schemes (see [66]). We refer the reader to [78] and [73] for detailed overviews of exact and approximation algorithms for different types of knapsack problems.

Objectives and assumptions. In this chapter, we depart from the assumption of a resourceful follower and study bilevel optimization in settings where the follower might use one of many algorithms to react to the upper-level decisions. In particular, we assume that the leader does not know upfront the algorithm to be used by the follower, but knows that it belongs to a known finite set of algorithms, which is denoted by $\mathcal{H}$. We refer to the uncertainty about the follower's choice of an algorithm from $\mathcal{H}$ as the *lower-level algorithmic uncertainty* or simply, the *lower-level uncertainty*. It is important to point out that in contrast to the stochastic and robust optimization methods that consider uncertainty issues related to the problem parameters and input data, our framework deals with uncertainty on the solution method used by the lower-level decision-maker, i.e., the follower.

Specifically, in our first modeling approach, we assume that the leader takes a conservative approach towards the lower-level uncertainty. That is, the leader assumes that, given an upper-level decision, the follower uses the algorithm from $\mathcal{H}$ that produces the most damaging (to the leader) lower-level decision.

In our second modeling approach we follow a less conservative method and assume that the follower instead selects the algorithm that produces a lower-level decision that is the Γ-th least damaging to the leader, where $\Gamma \in \{1, \ldots, |\mathcal{H}|\}$ is a parameter pre-defined by the decision-maker, i.e., the leader. Clearly, if $\Gamma = |\mathcal{H}|$, then both models coincide. By changing the value of Γ, the leader can control her level of conservatism, which is somewhat similar to the classical robust optimization approach of [21, 22] for dealing with data uncertainty in mathematical programming.

In our third modeling approach, we assume that the leader has prior information about the likelihood that the follower would use one of the algorithms, which is represented by a probability distribution over the set of possible algorithms. Using this information, the leader minimizes the expected value of her objective function, where the expectation is taken with respect to the follower's choice of an algorithm.

In developing our results we make several assumptions that are rather common in the bilevel optimization literature. In particular, we assume that the upper-level decisions are irrevocable and fully observed by the follower before selecting the lower-level decisions, and that the lower-level problem is well defined (i.e., it has a non-empty and bounded feasible region) for any possible set of upper-level decisions.

Furthermore, we assume that the leader knows the set of algorithms, $\mathcal{H}$, that might be used by the follower. Recall that in the standard bilevel optimization framework the leader has full information about the follower's optimization problem. Thus, it is reasonable to assume that the leader should be able to construct a set of algorithms $\mathcal{H}$ that contains one of the solution methods used by the follower. In this regard, traditional bilevel optimization can be seen through the lens of our framework when the follower always uses an exact algorithm that is, $\mathcal{H}$ consists of this algorithm and thus, $|\mathcal{H}| = 1$. Moreover, the optimistic and pessimistic models as well as the strong-weak approach ([31, 115]) of the standard bilevel optimization can also be viewed as special cases of our framework, see the discussion in Section 3.2.2.

Main contributions. Our contribution can be summarized as follows. First, we propose a framework that relaxes the assumption that the follower reacts optimally to the leader's decisions. This ought to fit settings where the follower either does not have the computational resources or is not sufficiently sophisticated to implement an exact approach to solve the lower-level problem. This is arguably the case in many application areas in practice, thus the approach contributes to closing the gap between the theory and practice in the bilevel optimization area. To the best of our knowledge, [103] is the only study in the bilevel optimization literature that studies a bilevel setting with an "*inexact*" follower, although in their network interdiction setting the follower uses one specific heuristic method, i.e., $|\mathcal{H}| = 1$, as opposed to selecting it from a set.

In this regard, we propose an approach to deal with the lower-level algorithmic uncertainty. We propose three different models to handling lower-level uncertainty that differ in their degree of conservatism and use of prior information on the likelihood of the use of any given algorithm by the follower. Furthermore, we propose different metrics to evaluate the (leader's) loss in the upper-level objective function due to the lower-level algorithmic uncertainty, that can be used to compare different approaches. In particular, we present a series of results that interconnect the different approaches towards uncertainty and the different metrics alluded above. These results allow quantifying and/or bounding upfront the leader's loss due to the lower-level uncertainty, and thus might be used in practice for selecting an appropriate approach to handling said uncertainty.

Second, we provide a prescriptive approach to the lower-level algorithmic uncertainty for a broad class of bilevel knapsack problems. In particular, we formulate the leader's (upper-level) problem when it is known that the follower selects its algorithm from a family of greedy approaches or implements an exact solution approach (see Section 3.4.2 for more details). We show that, in general, the upper-level problem remains NP-hard even when the follower is known to use a greedy method for solving the lower-level problem. Also, we provide a single-level mixed integer programming (MIP) formulation to the leader's decision problem. Single-level formulations of bilevel programs are common in settings where the lower-level problem admits a linear programming (LP) formulation. Remarkably, we obtain such a representation when the follower applies a greedy solution approach.

Finally, we illustrate our findings through numerical experiments on a specific class of bilevel knapsack problems. In particular, we consider a class of non-linear defender-attacker problems, which can be casted through the bilevel modeling framework (see [27] and references therein). We consider settings where the attacker might have limited computational resources and uses either an exact approach or one of two greedy-like approaches. Thus, our results illustrate the use of the proposed framework to help the leader in hedging against the lower-level algorithmic uncertainty in the context of defender-attacker problems.

Organization of this chapter. The next section provides some background material on bilevel optimization and presents the proposed modeling framework to address the lower-level algorithmic uncertainty, while Section 3.3 analyzes the leader's loss in performance. Section 3.4 presents our prescriptive approach to a broad class of bilevel knapsack problems. Section 3.5 presents a numerical study for the case of the defender-attacker model when the defender (leader) does not know the solution approach taken by the attacker (follower) but knows that it belongs to a family of greedy approaches. Finally, Section 3.6 presents our conclusions and final remarks.

3.2 MODELING FRAMEWORK FOR INEXACT FOLLOWER

In this chapter we consider a general class of bilevel mixed integer programs of the form

$$[\textbf{BMIP}]\ \min_{\mathbf{y}\in\mathcal{Y}} \quad f(\mathbf{y},\mathbf{x}) := g(\mathbf{y})^\top \mathbf{x} + t(\mathbf{y}) \tag{3.1a}$$

$$\text{subject to} \quad \mathbf{x} \in \mathcal{R}(\mathbf{y}) := \operatorname{argmax}\left\{c(\mathbf{y})^\top \hat{\mathbf{x}} \mid \hat{\mathbf{x}} \in \mathbb{X}(\mathbf{y})\right\}, \tag{3.1b}$$

where $\mathcal{Y} \subseteq \{0,1\}^{n_1-k_1} \times \mathbb{R}_+^{k_1}$ denotes the leader's feasible region, while $g, c : \mathcal{Y} \to \mathbb{R}^{n_2}$ and $t : \mathcal{Y} \to \mathbb{R}$. Set $\mathbb{X}(\mathbf{y}) \subseteq \{0,1\}^{n_2-k_2} \times \mathbb{R}_+^{k_2}$ denotes the follower's feasible region given leader's decision $y \in \mathcal{Y}$.

We refer to the minimization in (3.1a) as the upper-level problem, which is solved by the leader, and to the maximization on the right-hand-side of (3.1b) as the lower-level problem, which is solved by the follower. For each $\mathbf{y} \in \mathcal{Y}$, the set $\mathcal{R}(\mathbf{y}) \subseteq \{0,1\}^{n_2-k_2} \times \mathbb{R}_+^{k_2}$ is known as the *follower's rational reaction set*. The leader's and the follower's problems are general mixed integer programs (MIPs). Furthermore, if $k_1 = n_1$ and $k_2 = n_2$, g and c are constant vectors of appropriate dimensions, $t(\mathbf{y})$ is a linear function, and $\mathcal{Y} \times \mathbb{X}(\mathbf{y})$ is a polyhedral set, then **BMIP** reduces to a bilevel linear program (BLP). In contrast to the classical linear programming (LP) solvable in polynomial time, BLPs are NP-hard [38, 46].

In the remainder of this chapter we assume that:

Assumption A1: $\mathcal{Y}$ is non-empty and bounded.

Assumption A2: $\mathbb{X}(\mathbf{y})$ is non-empty and bounded for any $\mathbf{y} \in \mathcal{Y}$.

Assumptions **A1** and **A2** are typical in the bilevel optimization literature [38]. Whenever the lower-level problem has multiple optimal solutions for a given leader's decision, a "collaborative" follower might implement the solution that is the most favorable to the leader; on the other hand, an "adversarial" follower might select the most disadvantageous (to the leader) solution. These two situations are respectively referred to as the *optimistic* and *pessimistic* formulations of bilevel problems [38].

3.2.1 Inexact Follower

As outlined in Section 3.1, a key assumption in most studies in the bilevel optimization literature is that the follower's rational reaction set includes only optimal solutions of the lower-level problem (3.1b), see, e.g., some recent results in [18, 34, 45, 104]. However, in many application areas, given a leader's decision $\mathbf{y} \in \mathcal{Y}$, the resulting lower-level problem is NP-hard, which means that, in practice, an exact solution might not be found in a timely manner. Hence, in such settings the follower might use an approximate or heuristic solution instead, that are typically much faster to find.

Consider, for example, the aforementioned case of bilevel knapsack problems, where the lower-level problem takes the form of the linear 0–1 knapsack problem. Specifically, assume that for a given upper-level decision $\mathbf{y} \in \mathcal{Y}$, the lower-level problem is of the form:

$$\max \Big\{ \sum_i c_i x_i \mid \sum_i w_i x_i \leq b, \ \mathbf{x} \in \{0,1\}^{n_2} \Big\}. \tag{3.2}$$

While there exist multiple exact solution methods for the linear and nonlinear integer knapsack problems (e.g., dynamic programming or branch-and-bound based algorithms), there are also various approximation and heuristic methods [73]. One example is the popular *greedy* *method* that simply sorts the items in the non-increasing order of the ratio c_i/w_i, and selects the items prioritizing them according to said ratio, subject to the budgetary constraint. [1]

While heuristic and approximate approaches (as the greedy method above) for NP-hard problems (like knapsack problem) are ubiquitous in practice (see, e.g., examples in [55, 89]), most of the research studies in bilevel optimization typically ignore the follower's practical considerations. More importantly, ignoring such a choice might prevent the leader from anticipating the follower's actions and thus have profound consequences. To illustrate this point, we provide the following example.

Example 1. Consider a simple bilevel problem, which is an instance of **BMIP**:

$$\begin{aligned} \min_{\mathbf{y}\in\{0,1\}^2} \quad & f(\mathbf{y},\mathbf{x}) = y_1 + My_2 + x_1 + 2Mx_2 \\ \text{subject to} \quad & y_1 + y_2 = 1 \\ & \mathbf{x} \in \underset{\hat{\mathbf{x}}\in\{0,1\}^2}{\operatorname{argmax}} \, \{2M\hat{x}_1 + M\hat{x}_2 \;: M\hat{x}_1 + \hat{x}_2 \leq My_1\}, \end{aligned}$$

where M is a sufficiently large constant. Observe that the leader has two feasible solutions given by $\mathbf{y}^1 = (1,0)^\top$ and $\mathbf{y}^2 = (0,1)^\top$. If the follower solves his problem to optimality, then the leader's optimal solution is $\mathbf{y}^1 = (1,0)^\top$, which triggers the follower's reaction $\mathbf{x}^1 = (1,0)^\top$, resulting in the upper-level objective function value $f(\mathbf{y}^1,\mathbf{x}^1) = 2$. Next, consider a scenario where the follower uses the greedy heuristic based on the cost-to-weight ratio. If the leader implements $\mathbf{y}^1 = (1,0)^\top$, then the follower's response is $\mathbf{x}^2 = (0,1)^\top$. Consequently, the upper-level objective function value is $f(\mathbf{y}^1,\mathbf{x}^2) = 1 + 2M$. On the other hand, if the leader is aware of the fact that the follower applies the greedy heuristic, then she implements $\mathbf{y}^2 = (0,1)^\top$ resulting in the upper-level objective function value $f(\mathbf{y}^2,\mathbf{x}^3) = M$, where $\mathbf{x}^3 = (0,0)^\top$. Note that $f(\mathbf{y}^1,\mathbf{x}^2) - f(\mathbf{y}^2,\mathbf{x}^3) = M + 1$ and this difference between the resulting objective functions values can be made arbitrarily large. ■

In the remainder of this chapter, we assume that to find a solution to the lower-level problem the follower uses one of the algorithms from a pre-defined set $\mathcal{H}$. Formally, algorithm $h \in \mathcal{H}$ maps upper-level decisions to lower-level decisions and hence, is characterized

[1] It is worth mentioning that while the worst-case performance guarantee for the greedy method can be made arbitrarily close 0, a small variation of the algorithm provides a 1/2-approximation. [73, Chapter 2.5]

by the set of responses it produces (thus, two algorithms that reacts in the same way to all upper-level decisions are indistinguishable). Specifically:

Definition 1. *Follower's* reaction algorithm $h \in \mathcal{H}$ *is given by function* $\mathbf{x}^h(\cdot) : \mathcal{Y} \to \mathbb{R}^{n_2}$ *that maps an upper-level decision* $\mathbf{y} \in \mathcal{Y}$ *to a feasible lower-level decision* $\mathbf{x}^h(\mathbf{y})$ *in* $\mathbb{X}(\mathbf{y})$.

Note that by its definition, algorithm $h \in \mathcal{H}$ returns a *unique* feasible solution to the lower-level problem for every $\mathbf{y} \in \mathcal{Y}$, which is consistent with assumption **A2**. A key assumption in this work, which we formalize next, is that the leader does not know the algorithm that is used by the follower, but knows that it belongs to set $\mathcal{H}$ (recall our detailed discussion on justification of this assumption in Section 3.1).

Assumption A3: The reaction algorithm, h, used by the follower is not known to the leader in advance. However, the leader is aware of the set of possible reaction algorithms, $\mathcal{H}$, that is $h \in \mathcal{H}$.

Furthermore, in what follows, we make the distinction between *exact* and *inexact* algorithms. We say that $h \in \mathcal{H}$ is an exact algorithm if for any $\mathbf{y} \in \mathcal{Y}$ it returns an optimal solution to the lower-level problem, i.e., $\mathbf{x}^h(\mathbf{y}) \in \mathcal{R}(\mathbf{y})$. Similarly, we say $h \in \mathcal{H}$ is an inexact algorithm if it might return a suboptimal solution to the lower-level problem, i.e., there exists $\mathbf{y} \in \mathcal{Y}$ such that $\mathbf{x}^h(\mathbf{y}) \notin \mathcal{R}(\mathbf{y})$. For the linear knapsack 0–1 problem, for example, the aforementioned greedy method is, in general, an inexact algorithm. In addition, we say that algorithm h is *distinct* from h' if they return different solutions to some instance of the lower-level problem, i.e., there exists $\mathbf{y} \in \mathcal{Y}$ such that $\mathbf{x}^h(\mathbf{y}) \neq \mathbf{x}^{h'}(\mathbf{y})$. Note that both h and h' might be exact but distinct at the same time, which is possible whenever $\mathcal{R}(\mathbf{y})$ is not a singleton, for some $\mathbf{y} \in \mathcal{Y}$.

3.2.2 Approaches to the Lower-level Algorithmic Uncertainty

Next, we introduce modeling methods to handle the lower-level algorithmic uncertainty.

Robust Model (RBP). In this approach, the leader anticipates the worst possible outcome over $\mathcal{H}$. That is, the leader assumes that for any given upper-level decision, an adversarial follower uses the algorithm that damages the leader the most. Thus, the leader solves

$$[\mathbf{RBP}] \quad z^*_{\mathcal{H}} := \min_{\mathbf{y} \in \mathcal{Y}} \quad \max_{h \in \mathcal{H}} \quad f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) = g(\mathbf{y})^\top \mathbf{x}^h(\mathbf{y}) + t(\mathbf{y}). \tag{3.3}$$

Note that **RBP** can be viewed as a generalization of the pessimistic and optimistic cases of the standard bilevel optimization. For example, let h and h' be both exact algorithms for the follower's problem and assume that, for every $\mathbf{y} \in \mathcal{Y}$, algorithm h yields solutions that are most favorable for the leader, while h' returns the least favorable one: by setting $\mathcal{H} = \{h\}$ and $\mathcal{H} = \{h'\}$ in (3.3) we reduce **RBP** to either optimistic or pessimistic bilevel problems, respectively.

Γ-Robust Model (Γ-RBP). The approach in **RBP** can be seen as too conservative, especially when set $\mathcal{H}$ contains several solution methods. Next, we propose a more flexible model that enables the leader to control her level of conservatism. Let Γ be a positive integer representing the number of algorithms that the leader wishes to "hedge" against, i.e., $\Gamma \in \{1, \ldots, |\mathcal{H}|\}$. Then for a fixed value of Γ, the leader solves

$$[\mathbf{\Gamma\text{-}RBP}]\ z^*_\Gamma := \min_{S \subseteq \mathcal{H}, \mathbf{y} \in \mathcal{Y}, z} \left\{ z : f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) \leq z,\ \forall h \in S,\ \ |S| = \Gamma \right\}. \tag{3.4}$$

Note that in contrast to **RBP**, here the leader anticipates the Γ-th smallest realization among the follower's algorithms. Thus, **RBP** is a special case of **Γ-RBP** with $\Gamma = |\mathcal{H}|$. In other words, the leader minimizes the Γ-th smallest objective function among all values generated by the algorithms in $\mathcal{H}$. For example, for $\Gamma = 1$, the leader is effectively selecting the algorithm that the follower uses, while for $\Gamma = |\mathcal{H}|$, the leader anticipates that the follower uses the algorithm that hurts her the most, for any given upper-level decision. Simply speaking, in the **Γ-RBP** model the leader hedges against Γ algorithms from $\mathcal{H}$ and ignores $|\mathcal{H}| - \Gamma$ worst possible outcomes for her.

Hence, **Γ-RBP** can be re-written as the following mathematical program:

$$z^*_\Gamma := \min\ \rho \tag{3.5a}$$

$$\text{subject to} \quad \rho + M(1 - \sigma_h) \geq f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) \qquad \forall h \in \mathcal{H}, \tag{3.5b}$$

$$\sum_{h=1}^{|\mathcal{H}|} \sigma_h = \Gamma, \tag{3.5c}$$

$$\mathbf{y} \in \mathcal{Y},\ \sigma_h \in \{0, 1\}\ \forall h \in \mathcal{H}, \tag{3.5d}$$

where M is a sufficiently large constant parameter, e.g., $M := \max_{h \in \mathcal{H}, \mathbf{y} \in \mathcal{Y}} \{f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))\}$. In (3.5) we assume that such M exists. Note that the expression $f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))$ might not be readily available and itself might be the solution to a mathematical program.

Γ-RBP model is inspired by the robust optimization approach to matrix-data uncertainty in [21, 22]. In their works, the decision-maker hedges against any change to the matrix-data as long as it involves at most Γ changes to uncertain elements in the data matrix. In our work, the decision-maker instead hedges against the lower-level algorithmic uncertainty. In particular, in the **Γ-RBP** model, for a given upper-level decision, the leader anticipates that the follower uses the Γ-th most favorable (to her) algorithm in $\mathcal{H}$. According to intuition, the next result shows that the solution to **Γ-RBP** is non-decreasing in Γ.

Proposition 15. *The optimal objective function value of* **Γ-RBP**, z^*_Γ, *is non-decreasing in* Γ.

Proof. Given integer Γ, $1 \leq \Gamma \leq |\mathcal{H}|$, and any leader's feasible decision $\mathbf{y} \in \mathcal{Y}$, define

$$z_\Gamma(\mathbf{y}) := \min_{S,z} \left\{ z : f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) \leq z \quad \forall h \in S,\, S \subseteq \mathcal{H},\, |S| = \Gamma \right\},$$

and $z^*_\Gamma := \min_{\mathbf{y} \in \mathcal{Y}} \{z_\Gamma(\mathbf{y})\}$. Also, let $\mathbf{y}^*_\Gamma \in \mathcal{Y}$ denote the optimal solution to **Γ-RBP**, so that $z^*_\Gamma = z_\Gamma(\mathbf{y}^*_\Gamma)$. It follows that $z^*_\Gamma \leq z_\Gamma(\mathbf{y}^*_{\Gamma+1})$. Note now that, for every $S \subseteq S'$, one has that

$$\min \left\{ z : f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) \leq z \quad \forall h \in S \right\} \leq \min \left\{ z : f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) \leq z \quad \forall h \in S' \right\}.$$

Thus, $z_\Gamma(\mathbf{y}^*_{\Gamma+1}) \leq z_{\Gamma+1}(\mathbf{y}^*_{\Gamma+1}) = z^*_{\Gamma+1}$. The result follows from combining the above. ■

Proposition 15 formalizes the intuition that the leader's optimal objective function value deteriorates as she hedges against an increasing number of algorithms. As mentioned earlier, $\Gamma = |\mathcal{H}|$ corresponds to the most conservative follower, which is formalized by the following corollary.

Corollary 8. *For any integer* Γ *such that* $1 \leq \Gamma \leq |\mathcal{H}|$*:*

$$z^*_\Gamma \leq z^*_{|\mathcal{H}|} = z^*_{\mathcal{H}}$$

Example 2. Consider the following instance of a bilevel knapsack problem (see further discussion in Section 3.4):

$$\begin{aligned}
\min_{\mathbf{y}\in\mathbb{R}^4_+} \quad & (5-y_1)x_1 + (6-y_2)x_2 + (12-1.5y_3)x_3 + (17-2y_4)x_4 \\
\text{subject to} \quad & y_1+y_2+y_3+y_4 \le 10 \\
& \mathbf{x} \in \underset{\hat{\mathbf{x}}\in\{0,1\}^4}{\operatorname{argmax}}\ (3M-y_1)\hat{x}_1 + (100-0.5y_2)\hat{x}_2 + (90-y_3)\hat{x}_3 + (20-y_4)\hat{x}_4 \\
& \qquad \text{subject to} \quad M\hat{x}_1 + 50\hat{x}_2 + 30\hat{x}_3 + 21\hat{x}_4 \le M+50
\end{aligned}$$

Note that for a given leader's decision $\mathbf{y}$, the lower-level problem reduces to a knapsack binary problem of the form (3.2). Let $\mathcal{H}=\{h_1,\ h_2,\ h_3\}$ be three algorithms that the follower might use, where h_1 is an exact algorithm and h_2 is a greedy algorithm for solving 0–1 knapsack problem based on the c_i/w_i ratio (recall our earlier discussion in Section 3.1); furthermore, h_3 is also a greedy algorithm but the follower prioritizes items based on the value of w_i.

For sufficiently large value of M, regardless of the upper-level decision, the response of each algorithm in $\mathcal{H}$ is given by $\mathbf{x}^{h_1} = (1,1,0,0)^\top$, $\mathbf{x}^{h_2} = (1,0,1,0)^\top$ and $\mathbf{x}^{h_3} = (0,1,1,1)^\top$. Thus, for upper-level decision $\mathbf{y}^1 = (10,0,0,0)^\top$ we have that $f(\mathbf{y}^1,\mathbf{x}^{h_1}(\mathbf{y}^1)) = 1$, $f(\mathbf{y}^1,\mathbf{x}^{h_2}(\mathbf{y}^1)) = 7$ and $f(\mathbf{y}^1,\mathbf{x}^{h_3}(\mathbf{y}^1)) = 35$. Similarly, upper-level decision $\mathbf{y}^2 = (0,0,10,0)^\top$ results in $f(\mathbf{y}^2,\mathbf{x}^{h_1}(\mathbf{y}^2)) = 11$, $f(\mathbf{y}^2,\mathbf{x}^{h_2}(\mathbf{y}^2)) = 2$ and $f(\mathbf{y}^2,\mathbf{x}^{h_3}(\mathbf{y}^2)) = 20$. According to the **RBP** model, $\mathbf{y}^2$ is a better solution for the leader compared with $\mathbf{y}^1$ because $\max_h\{f(\mathbf{y}^2,\mathbf{x}^h(\mathbf{y}^2))\} = 20 \le \max_h\{f(\mathbf{y}^1,\mathbf{x}^h(\mathbf{y}^1))\} = 35$. If the leader applies the **Γ-RBP** model for $\Gamma = 2$, then $z_\Gamma(\mathbf{y}^1) = 7$ and $z_\Gamma(\mathbf{y}^2) = 11$, which implies that $\mathbf{y}^1$ is a better solution than $\mathbf{y}^2$ for $\Gamma = 2$ in **Γ-RBP**.

The optimal solution of **RBP** is $\mathbf{y}^*_{\mathcal{H}} = (0,0,1,9)^\top$, $z^*_{\mathcal{H}} = 15.5$ and z^*_Γ for different values of Γ is as follows: $z^*_{\Gamma=1} = 1$, $z^*_{\Gamma=2} = 5$ and $z^*_{\Gamma=3} = z^*_{\mathcal{H}}$. As expected from Proposition 15 and Corollary 8, we have: $z^*_{\Gamma=1} \le z^*_{\Gamma=2} \le z^*_{\Gamma=3} = z^*_{\mathcal{H}}$. ■

Probabilistic model (PBP). In **RBP** and **Γ-RBP** the leader does not use any prior information about the likelihood that the follower uses a particular algorithm. This type of information, if available, may help the leader to identify a better solution. Next, we suppose that the likelihood that the follower applies any given algorithm is available to the leader.

We assume that the leader uses this information to minimize her expected objective function value. That is, the leader solves

$$[\mathbf{PBP}]\ z_p^* = \min_{\mathbf{y}\in\mathcal{Y}} \quad \mathbb{E}_h[f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))] := \sum_{h\in\mathcal{H}} p_h f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})), \tag{3.6}$$

where p_h denotes the known probability that the follower uses algorithm $h \in \mathcal{H}$, i.e., $0 \leq p_h \leq 1$ and $\sum_{h\in\mathcal{H}} p_h = 1$.

Recall our earlier observation that the optimistic and pessimistic models of **BMIP** can be viewed as special cases of **RBP**. A similar generalization holds for **PBP**. Specifically, let methods h and h' be both exact algorithms for the follower's problem, but suppose that while h returns the solution that is most favorable for the leader, h' returns the least favorable one; then, for $\mathcal{H} = \{h, h'\}$ model **PBP** corresponds to a bilevel model, where the leader optimizes a convex combination of the leader's objective functions in the optimistic and pessimistic cases. Such setting has been considered in the bilevel optimization literature, mostly for bilevel linear programs, and is known as a *strong-weak* bilevel problem [1, 31, 115, 119].

In a sense, the strong-weak approach attempts to model settings with a partially collaborative follower, where the decision-maker knows the probabilities of cooperation or non-cooperation of the follower, respectively, i.e., the leader is not certain if the follower is either collaborative or adversarial, and thus attempts to make a robust decision by taking into account both situations. We note that the strong-weak model is a special case of **PBP**.

Proposition 16. *Let $z_{\mathcal{H}}^*$ and z_p^* be the optimal values of* **RBP** *and* **PBP***, respectively. Then $z_p^* \leq z_{\mathcal{H}}^*$.*

Proof. We have that

$$z_p^* = \min_{\mathbf{y}\in\mathcal{Y}} \ \mathbb{E}_{h\in\mathcal{H}}[f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))] \leq \mathbb{E}_{h\in\mathcal{H}}[f(\mathbf{y}_{\mathcal{H}}^*, \mathbf{x}^h(\mathbf{y}))] \leq \max_h \ f(\mathbf{y}_{\mathcal{H}}^*, \mathbf{x}^h(\mathbf{y})) = z_{\mathcal{H}}^*,$$

which implies the result. ∎

Example 3. Let $p = (p_{h_1}, p_{h_2}, p_{h_3}) = (0.3, 0.2, 0.5)$ in Example 2. Then, $\mathbf{y}_p^* = (0, 0, 10, 0)^\top$ and $z_p^* = 13.7$. Thus, we have $z_p^* = 13.7 \leq z_{\mathcal{H}}^* = 15.5$ which is aligned with Proposition 16.

■

The results of Proposition 16 have a simple intuitive interpretation. If the leader has some initial information (i.e., p_h for all $h \in \mathcal{H}$), then this information can be used to decrease her expected objective function value in comparison to the case when she needs to hedge against the worst possible outcome for her.

3.3 QUANTIFYING LEADER'S LOSS

In this section we explore the consequences, for the leader, of making erroneous assumptions about the follower's reaction method. For this, below we formally define the notion of the *leader's loss* and then explore its properties.

Let $\mathbf{y}^h$ denote the leader's optimal decision when the follower uses algorithm h, and let f_h^* be the leader's corresponding objective function value, i.e,

$$\mathbf{y}^h \in \underset{\mathbf{y} \in \mathcal{Y}}{\operatorname{argmin}} \{f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))\}, \quad f_h^* := f(\mathbf{y}^h, \mathbf{x}^h(\mathbf{y}^h)).$$

Definition 2. *The leader's loss for a decision* $\mathbf{y} \in \mathcal{Y}$ *and algorithm* $h \in \mathcal{H}$*, is given by:*

$$\Delta_h(\mathbf{y}) := f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) - f_h^* \tag{3.7}$$

Note that $\Delta_h(\mathbf{y}) \geq 0$ and $\Delta_h(\mathbf{y}^h) = 0$. Also, we define $\Delta_{hh'}$ as the leader's loss when the leader acts assuming that the follower uses algorithm h while he instead uses algorithm h'. That is,

$$\Delta_{hh'} := \Delta_{h'}(\mathbf{y}^h).$$

Using Definition 2, we can think of **PBP** as a model in which the leader minimizes her expected total loss. Indeed, we have that

$$\min_{\mathbf{y} \in \mathcal{Y}} \mathbb{E}_{h \in \mathcal{H}}[\Delta_h(\mathbf{y})] = \min_{\mathbf{y} \in \mathcal{Y}} \mathbb{E}_{h \in \mathcal{H}}[f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) - f_h^*] = \min_{\mathbf{y} \in \mathcal{Y}} \sum_{h \in \mathcal{H}} p_h f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})) - \sum_{h \in \mathcal{H}} p_h f_h^*, \tag{3.8}$$

which is equivalent to **PBP** as the second term in the right-hand side of (3.8) is a constant that is independent of the upper-level decision.

An alternative view of the leader's loss follows from comparing the realized upper-level objective function value with that anticipated by the leader.

Definition 3. *The ex-post (leader's) loss $\Delta^{\mathrm{A}}_{hh'}$ from anticipating the use of algorithm $h \in \mathcal{H}$ when the follower's response is actually computed using algorithm $h' \in \mathcal{H}$ is given by*

$$\Delta^{\mathrm{A}}_{hh'} = \max\left\{ f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f^*_h, 0 \right\} \tag{3.9}$$

Loosely speaking, the ex-post loss compares the objective function value attained with that expected. Thus, in some situations the follower might not react as anticipated but this results in an improvement in the leader's objective function value (relative to the value that would have been obtained were the follower to react as anticipated). In such situations the ex-post loss $\Delta^{\mathrm{A}}_{hh'}$ is zero. This situation is illustrated in the next example.

Example 4. Table 2 reports the leader's and the follower's optimal solutions for Example 2 given the same set of possible follower's solution methods. We compute the values of $\Delta^{\mathrm{A}}_{hh'}$ and $\Delta_{hh'}$ and represent them in matrices Δ^{A} and Δ. For example, we have that $\mathbf{y}^{h_1} = (10, 0, 0, 0)^\top$, $\mathbf{x}^{h_2}(\mathbf{y}^{h_1}) = (1, 0, 1, 0)^\top$, and $f(\mathbf{y}^{h_1}, \mathbf{x}^{h_2}(\mathbf{y}^{h_1})) = 7$. Thus, $\Delta^{\mathrm{A}}_{h_1h_2} = 7 - 1 = 6$, and $\Delta_{h_1h_2} = 7 - 2 = 5$. Furthermore:

$$\Delta^{\mathrm{A}} = \begin{bmatrix} 0 & 6 & 34 \\ 9 & 0 & 18 \\ 0 & 2 & 0 \end{bmatrix}; \qquad \Delta = \begin{bmatrix} 0 & 5 & 20 \\ 10 & 0 & 5 \\ 10 & 15 & 0 \end{bmatrix}.$$

■

The following lemmas establish some logical relationships between loss and ex-post loss.

Lemma 3. *For any pair of algorithms $h, h' \in \mathcal{H}$ one has that $f^*_h \geq f^*_{h'} \Leftrightarrow \Delta^{\mathrm{A}}_{hh'} \leq \Delta_{hh'}$, and $f^*_h \leq f^*_{h'} \Rightarrow \Delta^{\mathrm{A}}_{hh'} \geq \Delta_{hh'}$.*

Table 2: Optimal solutions for different follower's reaction methods in Example 2.

h	$\mathbf{x}^h$	$\mathbf{y}^h$	f_h^*
h_1	$(1,1,0,0)^\top$	$(10,0,0,0)^\top$	1
h_2	$(1,0,1,0)^\top$	$(0,0,10,0)^\top$	2
h_3	$(0,1,1,1)^\top$	$(0,0,0,10)^\top$	15

Proof. ($\Rightarrow$) First, consider the case when $f_h^* \leq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h))$. In this case we have that $f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_{h'}^* \geq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_h^* \geq 0$, which implies directly that $\Delta_{hh'}^{\mathrm{A}} \leq \Delta_{hh'}$. Suppose now that $f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) \leq f_h^*$. Then $\Delta_{hh'}^{\mathrm{A}} = 0$, and the results follows from the fact that $\Delta_{hh'} \geq 0$.

($\Leftarrow$) First, consider the case when $\Delta_{hh'}^{\mathrm{A}} > 0$: we have that

$$\Delta_{hh'}^{\mathrm{A}} \leq \Delta_{hh'} \;\Rightarrow\; f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_h^* \leq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_{h'}^* \;\Rightarrow\; f_{h'}^* \leq f_h^*.$$

Suppose now that $\Delta_{hh'}^{\mathrm{A}} = 0$, then $f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) \leq f_h^*$ and we have that $f_{h'}^* \leq f_h^*$ because of the optimality of $\mathbf{y}^{h'}$. With regard to the second assertion in the statement of the lemma, we have

$$\Delta_{hh'}^{\mathrm{A}} \geq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_h^* \geq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_{h'}^* = \Delta_{hh'},$$

where the first inequality holds by the definition of $\Delta_{hh'}^{\mathrm{A}}$ and the second inequality follows from the assumption that $f_h^* \leq f_{h'}^*$. ■

Lemma 4. *For any pair of algorithms $h, h' \in \mathcal{H}$, if $\Delta_{hh'}^{\mathrm{A}} = 0$, then $f_{h'}^* \leq f_h^*$ and $\Delta_{hh'} \leq f_h^* - f_{h'}^*$.*

Proof. If $\Delta_{hh'}^{\mathrm{A}} = 0$, then $f_{h'}^* \leq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) \leq f_h^*$ which proves the first part of the lemma. The second part follows directly from this and the definition of $\Delta_{hh'}$. ■

Lemma 4 provides an upper bound for $\Delta_{hh'}$ when the upper-level objective function value is not larger than anticipated. Note that $\Delta_{hh'}^{\mathrm{A}} = 0$ does not necessarily imply $\Delta_{hh'} = 0$, which is illustrated further in Example 5 below. In other words, if the leader obtains the value smaller or equal to what anticipated, then this does not imply that the leader has implemented the best possible decision.

The next proposition provides a bound on the objective function value attained by the leader when implementing the solution prescribed by **RBP** for $|\mathcal{H}| = 2$.

Proposition 17. *Suppose that* $\mathcal{H} = \{h, h'\}$*. Then*

$$z^*_{\mathcal{H}} \leq \min\left\{f^*_h + \Delta^{\mathrm{A}}_{hh'}, f^*_{h'} + \Delta^{\mathrm{A}}_{h'h}\right\}. \tag{3.10}$$

Moreover, if $\Delta^{\mathrm{A}}_{hh'} = 0$*, then* $z^*_{\mathcal{H}} = f^*_h$*.*

Proof. Let $\mathbf{y}^*_{\mathcal{H}}$ denote an optimal solution to **RBP**. We have that

$$z^*_{\mathcal{H}} = \min_{\mathbf{y}\in\mathcal{Y}} \max\left\{f(\mathbf{y}, \mathbf{x}^h(\mathbf{y})), f(\mathbf{y}, \mathbf{x}^{h'}(\mathbf{y}))\right\} \leq \max\{f^*_h, f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h))\},$$

where the inequality follows as $\mathbf{y}^h \in \mathcal{Y}$. Recalling that $z^*_{\mathcal{H}} = \max\{f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^h(\mathbf{y}^*_{\mathcal{H}})), f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h'}(\mathbf{y}^*_{\mathcal{H}}))\}$, we have that

$$f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h'}(\mathbf{y}^*_{\mathcal{H}})) \leq z^*_{\mathcal{H}} \leq \max\{f^*_h, f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h))\} = f^*_h + \Delta^{\mathrm{A}}_{hh'},$$

where the last equality holds by the definition of $\Delta^{\mathrm{A}}_{hh'}$. With regard to the second assertion in the statement, we have (from above) that $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^h(\mathbf{y}^*_{\mathcal{H}})) \leq z^*_{\mathcal{H}}$. Because $\Delta^{\mathrm{A}}_{hh'} = 0$, we obtain $f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) \leq f^*_h$ from the first part of this proof. Hence, we have that

$$f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^h(\mathbf{y}^*_{\mathcal{H}})) \leq z^*_{\mathcal{H}} \leq \max\left\{f^*_h, f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h))\right\} = f^*_h \leq f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^h(\mathbf{y}^*_{\mathcal{H}})),$$

and the result follows. ∎

Proposition 17 allows us to compare **RBP** with **BMIP** when $|\mathcal{H}| = 2$. In particular, we see that when $\Delta^{\mathrm{A}}_{hh'} = 0$ both problems have the same optimal objective function value. However, if $\Delta^{\mathrm{A}}_{hh'} > 0$, then inequality (3.10) reduces to $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h'}(\mathbf{y}^*_{\mathcal{H}})) \leq f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h))$. Thus, if the follower uses algorithm h', then the leader is better of implementing an optimal solution of **RBP**, $\mathbf{y}^*_{\mathcal{H}}$ rather than $\mathbf{y}^h$. This observation is rather natural as it is implied by the intuition behind model **RBP**. Note that Example 5 below illustrates the fact that

$z^*_{\mathcal{H}} = f^*_h$ does not necessarily indicate that $f^*_h = f^*_{h'}$. Also, some of the structural properties are illustrated in this example.

The next corollary, which we state without proof, establishes an upper bound for $z^*_{\mathcal{H}}$ in terms of $\Delta_{hh'}$ instead of $\Delta^A_{hh'}$.

Corollary 9. *Suppose that $\mathcal{H} = \{h, h'\}$. If $\Delta^{\mathrm{A}}_{hh'} \geq 0$ and $\Delta^{\mathrm{A}}_{h'h} \geq 0$, then*

$$z^*_{\mathcal{H}} \leq \min\left\{f^*_{h'} + \Delta_{hh'}, f^*_h + \Delta_{h'h}\right\}.$$

Example 5. Based on the information provided in Table 2 and Example 4, $f^*_{h_1} \leq f^*_{h_2}$ and $\Delta^{\mathrm{A}}_{h_1h_2} \geq \Delta_{h_1h_2}$. This is consistent with Lemma 3. Moreover, $\Delta^{\mathrm{A}}_{h_3h_1} = 0$ and $\Delta_{h_3h_1} = 10$ which reflects the fact that $\Delta^{\mathrm{A}}_{h_3h_1} = 0$ does not necessarily result in $\Delta_{h_3h_1} = 0$. In addition, $\Delta_{h_3h_1} = 10 \leq f^*_{h_3} - f^*_{h_1} = 15 - 1$ and it illustrates Lemma 4. Next, we show that $z^*_{\mathcal{H}} = f^*_{h_1}$ does not necessarily imply that $f^*_{h_1} = f^*_{h_2}$. Let $\mathcal{H} = \{h_1, h_2\}$, and if the coefficient of x_3 in the leader's objective function is changed from $(12 - 1.5y_3)$ to $(6 - 1.1y_3)$, then $\Delta^{\mathrm{A}}_{h_1h_2} = 0$ and $z^*_{\mathcal{H}} = f^*_{h_1} = 1$. However, $f^*_{h_2} = 0 \neq f^*_{h_1}$.

Finally, for $\mathcal{H} = \{h_1, h_2\}$ in Example 2, $\mathbf{y}^*_{\mathcal{H}} = (6, 0, 4, 0)^\top$ and $z^*_{\mathcal{H}} = 5$. According to Proposition 17, $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h_2}(\mathbf{y}^*_{\mathcal{H}})) \leq f^*_{h_1} + \Delta^{\mathrm{A}}_{h_1h_2}$, i.e., $5 \leq 1 + 6$, and $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h_1}(\mathbf{y}^*_{\mathcal{H}})) \leq f^*_{h_2} + \Delta^{\mathrm{A}}_{h_2h_1}$, i.e., $5 \leq 2 + 9$. Similarly, based on Corollary 9, $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h_2}(\mathbf{y}^*_{\mathcal{H}})) \leq f^*_{h_2} + \Delta_{h_1h_2}$, i.e., $5 \leq 2 + 5$, and $f(\mathbf{y}^*_{\mathcal{H}}, \mathbf{x}^{h_1}(\mathbf{y}^*_{\mathcal{H}})) \leq f^*_{h_1} + \Delta_{h_2h_1}$, i.e., $5 \leq 1 + 10$. ■

The results in Proposition 17 can be extended for the optimal solution of **PBP**, as shown next.

Proposition 18. *Suppose that $\mathcal{H} = \{h, h'\}$ and that $p_{h'} > 0$ and $p_h > 0$. We have that*

$$z^*_p \leq p_{h'}(f^*_{h'} + \Delta_{hh'}) + p_h(f^*_h + \Delta_{h'h}) \tag{3.11}$$

Proof. Let $\mathbf{y}^*_p$ denote an optimal solution of **PBP**. First, note that both terms $p_h\Big(f(\mathbf{y}^*_p, \mathbf{x}^h(\mathbf{y}^*_p)) - f^*_h\Big)$ and $p_{h'}\Big(f(\mathbf{y}^*_p, \mathbf{x}^{h'}(\mathbf{y}^*_p)) - f^*_{h'}\Big)$ are non–negative. Therefore, we have that

$$p_{h'}\Big(f(\mathbf{y}^*_p, \mathbf{x}^{h'}(\mathbf{y}^*_p)) - f^*_{h'}\Big) \leq p_h\Big(f(\mathbf{y}^*_p, \mathbf{x}^h(\mathbf{y}^*_p)) - f^*_h\Big) + p_{h'}\Big(f(\mathbf{y}^*_p, \mathbf{x}^{h'}(\mathbf{y}^*_p)) - f^*_{h'}\Big).$$

From the optimality of $\mathbf{y}_p^*$ to (3.8), we have that

$$p_h\Big(f(\mathbf{y}_p^*, \mathbf{x}^h(\mathbf{y}_p^*)) - f_h^*\Big) + p_{h'}\Big(f(\mathbf{y}_p^*, \mathbf{x}^{h'}(\mathbf{y}_p^*)) - f_{h'}^*\Big)$$
$$\leq p_h\Big(f(\mathbf{y}^h, \mathbf{x}^h(\mathbf{y}^h)) - f_h^*\Big) + p_{h'}\Big(f(\mathbf{y}^h, \mathbf{x}^{h'}(\mathbf{y}^h)) - f_{h'}^*\Big) = p_{h'}\Delta_{hh'},$$

which implies $p_{h'}\Big(f(\mathbf{y}_p^*, \mathbf{x}^{h'}(\mathbf{y}_p^*)) - f_{h'}^*\Big) \leq p_{h'}\Delta_{hh'}$, that is, $f(\mathbf{y}_p^*, \mathbf{x}^{h'}(\mathbf{y}_p^*)) \leq f_{h'}^* + \Delta_{hh'}$. The result follows from exchanging the role of h and h' above and considering the weighted sum.

■

3.4 BILEVEL KNAPSACK PROBLEM

In this section we apply the framework developed in Sections 3.2 and 3.3 to a special class of **BMIP** known as the bilevel knapsack problem (**BKP**), which can be written in the following form:

$$[\mathbf{BKP}] \ \min_{\mathbf{y}} \ f(\mathbf{y},\mathbf{x}) := \sum_{i=1}^{n_2} \big(g_{i0} + \sum_{j=1}^{n_1} g_{ij} y_j\big) x_i + \sum_{j=1}^{n_1} t_j y_j \tag{3.12a}$$

$$\text{subject to} \quad \mathbf{y} \in \mathcal{Y} := \{\mathbf{y} : \ A\mathbf{y} \leq b, \mathbf{y} \in \{0,1\}^k \times \mathbb{R}_+^{n_1-k}\}, \tag{3.12b}$$

$$\mathbf{x} \in \mathcal{R}(\mathbf{y}) := \quad \underset{\hat{\mathbf{x}} \in \{0,1\}^{n_2}}{\text{argmax}} \left\{ \sum_{i=1}^{n_2} \big(c_{i0} + \sum_{j=1}^{n_1} c_{ij} y_j\big) \hat{x}_i : w^\top \hat{\mathbf{x}} \leq d \right\}, \tag{3.12c}$$

where $A \in \mathbb{R}^{m\times n_1}$, $b \in \mathbb{R}^{m\times 1}$, $w \in \mathbb{R}_{>0}^{n_2\times 1}$, $d \in \mathbb{R}_{>0}^1$. Note that the functions $g_i(\cdot)$, $c_i(\cdot)$ and $t(\cdot)$ are affine with respect to $\mathbf{y}$, where $g_{i0}, \ g_{ij}, \ c_{i0}, \ c_{ij}, \ t_j \in \mathbb{R}$ for all $i \in \{1, \ldots, n_2\}$ and $j \in \{1, \ldots, n_1\}$. In order to simplify the notation, our definition of **BKP** contemplates a single constraint in the follower's knapsack problem. However, the prescriptive approach offered in this section admits a rather straightforward generalization to multiple constraints.

BKP is used to illustrate the proposed framework for two reasons. First, the bilevel knapsack problem (3.12) and its variants form a well-known class of bilevel optimization problems (see, e.g., [18, 26, 32, 33, 43, 86]). In particular, our numerical examples in Section 3.5 are based on a special class of **BKP** that has military and law-enforcement applications in the context of the defender-attacker models. The second reason is that, for any upper-level decision $\mathbf{y} \in \mathcal{Y}$, the follower's problem reduces to a linear 0–1 knapsack problem, which is known to be NP-hard [54]. The 0–1 knapsack problem is one of the most studied combinatorial optimization problems, mainly because of its simple integer programming formulation, its recurrent appearance in the study of more complex problems, and its capability of representing various real-life decision situations [78]. More importantly, in practical settings, the 0–1 knapsack problem is often solved by applying greedy heuristic approaches (recall our earlier examples in the previous sections): see Section 3.4.2 for a detailed discussion.

In what follows, we assume that each algorithm in $\mathcal{H}$ fulfills minimum *local optimality* conditions.

Assumption A4: For any $h \in \mathcal{H}$ we have that: (i) if the i^{th} component of $c(\mathbf{y})$ is non-positive, then $x_i^h(\mathbf{y}) = 0$, $i = 1, \ldots, n_2$; and (ii) if $x_i^h(\mathbf{y}) = 0$, then $\tilde{\mathbf{x}}^h(\mathbf{y}) = (x_1^h, \ldots, x_{i-1}^h, 1, x_{i+1}^h, \ldots, x_{n_2}^h)$ is infeasible, i.e., $w^\top \tilde{\mathbf{x}}^h(\mathbf{y}) > d$.

Assumption **A4** states that algorithms in $\mathcal{H}$ do not pack items with clearly unfavorable costs, and do not generate solutions that can be easily improved by adding a single item. Next, we show that when Assumption **A4** holds, **BKP** remains NP-hard even if the follower applies an inexact solution algorithm from $\mathcal{H}$.

Proposition 19. BKP *remains NP–hard when the maximization on the r.h.s. of* (3.12c) *is solved using any algorithm h for which* **A4** *holds.*

Proof. Consider the SUBSET SUM problem, which is known to be NP-complete [54]. Given a set of positive integers $S = \{s_1, \ldots, s_n\}$ and a positive integer $k \leq \sum_{i=1}^n s_i$, the SUBSET SUM problem consists of deciding whether or not there exists a subset $\tilde{S} \subseteq S$ such that $\sum_{i \in \tilde{S}} s_i = k$. Consider the following instance of **BKP**:

$$f^* = \min_{\mathbf{y} \in \{0,1\}^n} f(\mathbf{y}, \mathbf{x}^h(y)) = -\sum_{i=1}^n s_i y_i x_i^h(y), \tag{3.13}$$

where $\mathbf{x}^h(y)$ denotes a solution provided by algorithm h for

$$\max_{\mathbf{x} \in \{0,1\}^n} \Big\{ \sum_{i=1}^n s_i y_i x_i : \sum_{i=1}^n s_i x_i \leq k \Big\}.$$

The follower's constraint implies that $f^* \geq -k$. If SUBSET SUM problem has a solution, i.e., there exists subset $\tilde{S} \subseteq S$ such that $\sum_{i \in \tilde{S}} s_i = k$, then the leader's optimal solution is $y_i = 1$ for all $i \in \tilde{S}$ and $y_i = 0$, otherwise. In this case, under Assumption **A4**, the follower's response, based on any algorithm $h \in \mathcal{H}$, is $x_i^h = 1$ if $i \in \tilde{S}$ and $x_i^h = 0$, otherwise.

On the other hand, if an optimal solution of (3.13) results in $f^* = -k$, then $\tilde{S} = \{s_i : y_i = x_i = 1\}$ corresponds to a "yes" answer of the SUBSET SUM problem. Thus, SUBSET SUM problem has a solution *iff* $f^* = -k$. ■

It is worth noting that Proposition 19 holds for any set of approximation and heuristics algorithms, as long as Assumption **A4** holds. This result can be extended to the other proposed formulations. We formalize this in the following corollary, which we state without proof.

Corollary 10. **RBP**, **PBP** *and* **BMIP** *for any fixed* $\Gamma \in \{1, \ldots, |\mathcal{H}|\}$*, are* NP*-hard.*

Next, we introduce a family of greedy algorithms for solving the linear 0–1 knapsack problem and present a single-level formulation of **BKP** for selecting the upper-level decisions when the follower uses one of such greedy methods. Before that, we briefly discuss the case when the follower uses an exact algorithm to solve the lower-level problem (we use such a model in the numerical experiments in Section 3.5).

3.4.1 BKP with an exact follower

Consider the case of an exact follower, i.e., we assume that $\mathcal{H} = \{h\}$, with h exact. We briefly describe a cutting plane algorithm for solving **BKP** based on its single-level relaxation. Specifically, the latter is given by the problem of the form:

$$
\begin{aligned}
[\mathbf{SKP}] \quad \min_{\mathbf{y},\mathbf{x}} \ f(\mathbf{y},\mathbf{x}) := & \sum_{i=1}^{n_2} \big(g_{i0} + \sum_{j=1}^{n_1} g_{ij} y_j\big) x_i + \sum_{j=1}^{n_1} t_j y_j \\
\text{subject to} \quad & A\mathbf{y} \leq b, \\
& w^\top \mathbf{x} \leq d, \\
& \mathbf{y} \in \{0,1\}^k \times \mathbb{R}_+^{n_1 - k}, \ \mathbf{x} \in \{0,1\}^{n_2},
\end{aligned}
$$

where a single decision-maker controls both sets of decision variables and the follower's objective function is completely disregarded. Thus, **SKP** is a single-level mathematical program and referred to as a single-level relaxation of **BKP**.

Clearly, the optimal objective function value of **SKP** provides a lower bound for the optimal objective function value of **BKP**. Note that solution approaches based on exploiting single-level relaxations as bounding mechanisms are among the most common approaches in the bilevel optimization literature, see, e.g., a recent example in [34] for solving bilevel linear integer problems. In this section, we demonstrate an application of this approach for a class of nonlinear bilevel problem given by **BKP**.

In particular, we observe that **SKP** is a nonlinear mixed integer problem due to the presence of nonlinear terms $y_j x_i$ in its objective function. However, these terms can be linearized by introducing new variables z_{ij} and additional set of linear constraints (see, further details and discussion in [2]):

$$\left\{(x_i, y_j, z_{ij})\colon z_{ij} = y_j x_i,\ x_i \in \{0,1\},\ y_j^L \leq y_j \leq y_j^U\right\} =$$
$$\left\{(x_i, y_j, z_{ij})\colon x_i \in \{0,1\},\ z_{ij} \leq y_j^U x_i,\ z_{ij} \leq y_j + y_j^L x_i - y_j^L,\ z_{ij} \geq y_j^L x_i,\ z_{ij} \geq y_j + y_j^U x_i - y_j^U\right\},$$

where we assume that the lower (y_j^L) and upper (y_j^U) bounds on y_j for each $j \in \{1, \ldots, n_1\}$ are either readily available or can be easily computed. (The bounds exist due to Assumption **A1**: note that tighter bounds could improve solution times). Hence, **SKP** can be re-written as an equivalent linear MIP that can be solved by a standard solver. This observation also implies that **SKP** has a finite optimal solution.

The pseudo-code of the exact cutting-plane based approach for solving **BKP** is provided in Algorithm 1, whose convergence is established in the next result.

Proposition 20. *Algorithm 1 outputs an optimal solution of* **BKP** *in a finite number of iterations.*

Proof. Because $\check{\mathbf{x}}$ is a binary vector, the number of cuts of the form presented at **Step 3** is finite. Thus, it is sufficient to show that a cut at **Step 3** is never regenerated.

Let $(\hat{\mathbf{y}}^\kappa, \hat{\mathbf{x}}^\kappa)$ be the optimal solution of **SKP** after adding the κ-th cut and $\check{\mathbf{x}}^\kappa$ be the follower's optimal solution for $\mathbf{y} = \hat{\mathbf{y}}^\kappa$. If $\sum_{i=1}^{n_2} \big(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j\big)\check{x}_i = \sum_{i=1}^{n_2} \big(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j\big)\hat{x}_i$,

Algorithm 1 Exact Algorithm for solving **BKP**

Step 1. Solve **SKP** and denote by $(\hat{\mathbf{y}}, \hat{\mathbf{x}})$ its optimal solution.

Step 2. Solve linear binary problem (3.12c) for $\mathbf{y} = \hat{\mathbf{y}}$. Let $\check{\mathbf{x}}$ and z_f^* denote its optimal solution and the optimal objective function value, respectively.

if $z_f^* = \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j\right)\hat{x}_i$ **then**

$(\hat{\mathbf{y}}, \hat{\mathbf{x}})$ is an optimal solution of **BKP**; **STOP**.

end if

if $z_f^* > \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j\right)\hat{x}_i$ **then**

Go to **Step 3**.

end if

Step 3. Add a linear constraint of the form:

$\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}y_j\right)x_i \geq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}y_j\right)\check{x}_i$ to **SKP** and go to **Step 1**.

then Algorithm 1 stops according to **Step 2**. Otherwise, we add $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}y_j\right)x_i \geq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}y_j\right)\check{x}_i^\kappa$ to **SKP**. Let $(\hat{\mathbf{y}}^{\kappa+1}, \hat{\mathbf{x}}^{\kappa+1})$ be its optimal solution in the next iteration. Then we have two possible situations:

(i) If $\hat{\mathbf{y}}^{\kappa+1} = \hat{\mathbf{y}}^\kappa$, then $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\hat{x}_i^{\kappa+1} \geq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\check{x}_i^\kappa$. We also know that $\check{\mathbf{x}}^\kappa$ is the follower's optimal solution for $\mathbf{y} = \hat{\mathbf{y}}^\kappa$, i.e., $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\hat{x}_i^{\kappa+1} \leq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\check{x}_i^\kappa$. Thus, $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\hat{x}_i^{\kappa+1} = \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^\kappa\right)\check{x}_i^\kappa$. That is $(\hat{\mathbf{y}}^{\kappa+1}, \hat{\mathbf{x}}^{\kappa+1})$ is an optimal solution for **BKP** and the algorithm stops.

(ii) If $\hat{\mathbf{y}}^{\kappa+1} \neq \hat{\mathbf{y}}^\kappa$, then let $\check{\mathbf{x}}^{\kappa+1}$ be the follower's optimal solution for $\mathbf{y} = \hat{\mathbf{y}}^{\kappa+1}$. We have $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\hat{x}_i^{\kappa+1} \leq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\check{x}_i^{\kappa+1}$ and $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\hat{x}_i^{\kappa+1} \geq \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\check{x}_i^\kappa$. Thus, if $\check{\mathbf{x}}^{\kappa+1} = \check{\mathbf{x}}^\kappa$, then $\sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\hat{x}_i^{\kappa+1} = \sum_{i=1}^{n_2} \left(c_{i0} + \sum_{j=1}^{n_1} c_{ij}\hat{y}_j^{\kappa+1}\right)\check{x}_i^{\kappa+1}$, which implies that $(\hat{\mathbf{y}}^{\kappa+1}, \hat{\mathbf{x}}^{\kappa+1})$ is an optimal solution of **BKP** and the algorithm stops. Otherwise, $\check{\mathbf{x}}^{\kappa+1} \neq \check{\mathbf{x}}^\kappa$ and the algorithm generates a new cut. ■

Exact solution approaches based on single-level relaxations along with cutting plane and/or branch-and-bound based ideas are very common in the bilevel literature (see, e.g.

[8, 10, 34, 45]). While the vast majority of such approaches focus on linear or linear mixed integer bilevel problems, our model contains nonlinear terms. More importantly, this cutting plane algorithm can be extended to solve models from Section 3.2.2, see our discussion next.

3.4.2 BKP with a greedy follower

3.4.2.1 The greedy follower. The 0–1 knapsack problem, one of the most studied combinatorial problems, can not be solved in polynomial time (unless $P = NP$). However, because of its relevance to practice, multiple exact and approximate solution algorithms have been proposed, many of which are used in practice.

In this section, we focus our analysis on a simple version of the greedy algorithm, see [73]. In its simplest form, the greedy algorithm first ranks the available alternatives (referred to as items in the context of knapsack problems) based on their *cost-to-weight* ratio c_i/w_i, where

$$c_i \equiv c_i(\mathbf{y}) = c_{i0} + \sum_{j=1}^{n_1} c_{ij} y_j,$$

and then goes through the ranking (in decreasing order, so items with greater ranking are preferred), selecting items if their inclusion does not violate the capacity constraint $w^\top \mathbf{x} \leq d$.

More generally, the follower may use different *rating functions* (besides the cost-to-weight ratio) in a hierarchical fashion to rank items (so that ties in the overall ranking are broken using ratings hierarchically), see, e.g., [63]. In what follows, we use such a generalization of the greedy algorithm.

Specifically, we say that a rating function $r := (r_i(c_i, w_i), i = 1, \ldots, n_2) \in \mathbb{R}^{n_2}$ assigns rating $r_i \equiv r_i(c_i, w_i) \in [0, 1]$ to item i, which is a function of its cost and weight. We consider a set of rating functions $\{r^1, \ldots, r^K\}$ for some positive integer K. Define $\mathcal{K} := \{1, \ldots, K\}$ and

$$k_{ij} := \operatorname{argmax}\{k \ : \ r_i^\ell = r_j^\ell \text{ for all } \ell < k, \ k \in \mathcal{K}\} \tag{3.15}$$

for any pair of distinct items (i, j), where $r_i^0 = 0$ for all i.

Let "$\succ$" denote the *preference* relation among items, i.e., $i \succ j$ denotes that i is preferred (regarding selection) over j. The preference relationship is such that

$$r_i^{k_{ij}} > r_j^{k_{ij}} \quad \Longleftrightarrow \quad i \succ j.$$

Note that by (3.15) there may exist a tie in rankings between i and j if and only if $k_{ij} = K$ and $r_i^K = r_j^K$. For simplicity of exposition we assume that such scenarios do not occur.

The above discussion implies that ratings are used in a lexicographic fashion to define the overall ranking. That is, rankings r^1, ..., r^K are ordered according to the follower's preferences. With the above, we assume that, for $\mathbf{y}$ given, the follower solves (3.12c) using the *Greedy Heuristic* described below.

Algorithm 2 Greedy Heuristic

Step 1: Order items according to "$\succ$." Relabel items so that $i \succ i+1$ for all i. Let $i \leftarrow 1$.

Step 2: Pick item i if its selection does not violate the knapsack constraint. Let $i \leftarrow i+1$.

Step 3: If $i \leq n_2$, go to **Step 2**. Otherwise, return the obtained solution.

3.4.2.2 Single-level MIP reformulation. Single-level reformulations for bilevel programs are common in settings where the lower-level problem admits an LP formulation (see, e.g., [9] and [114]). In particular, the strong duality property of LPs is usually exploited to derive single-level MIP reformulations that can be handled by standard MIP solution methods. For more complex lower-level problems (e.g., general MIPs at the lower level) single-level reformulations are not typically available (at least not polynomially sized) when the follower uses an exact algorithm. Next, we leverage the structure of the follower's greedy heuristic to provide a single-level reformulation of **BKP** with irrational follower.

Decision variables. Let $N = \{1, \dots, n_2\}$. For item $i \in N$, let binary variable x_i represent the selection of item i, i.e.

$$x_i = \begin{cases} 1 & \text{if item } i \text{ selected,} \\ 0 & \sim . \end{cases}$$

We consider following binary variables for distinct items i and j: α_{ij} represents whether $i \succ j$; q_{ij} denotes if $i \succ j$ and item i is selected; and z_{ij}^k signals whether there is a tie in the k-th rating function between items i and j. This is,

$$\alpha_{ij} = \begin{cases} 1 & \text{if } i \succ j, \\ 0 & \sim, \end{cases}, \quad q_{ij} = \alpha_{ij}\, x_i, \quad z^k_{ij} = \begin{cases} 1 & \text{if } r^k_i = r^k_j, \\ 0 & \sim . \end{cases}$$

Constraints. First, we force preferences to align with the set of rating functions. Thus, we begin ordering items using ranking function r^1 by considering the following set of constraints.

$$r^1_i \leq r^1_j + \alpha_{ij} \qquad \forall i, j \in N \tag{3.16a}$$

$$\alpha_{ij} + \alpha_{ji} = 1 \qquad \forall i, j \in N \tag{3.16b}$$

$$q_{ij} \leq \alpha_{ij} \qquad \forall i, j \in N \tag{3.16c}$$

$$\sum\nolimits_{j=1}^{n} q_{ij} \leq n x_i \qquad \forall i \in N \tag{3.16d}$$

$$\alpha_{ij} + x_i \leq q_{ij} + 1 \qquad \forall i, j \in N \tag{3.16e}$$

Constraints (3.16a)-(3.16b) provide consistency to the value of α_{ij}, when $r^1_i \neq r^1_j$. Constraints (3.16c)–(3.16e) assure that q_{ij} is equal to x_i when $i \succ j$, and zero otherwise.

When $r^1_i = r^1_j$, we require α_{ij} to be consistent with the remaining rating functions. We do this via the following set of constraints.

$$-(1 - z^k_{ij}) \leq r^k_i - r^k_j \leq (1 - z^k_{ij}) \qquad \forall i, j \in N, k \in \mathcal{K} \tag{3.17a}$$

$$r^k_j - r^k_i \leq \sum\nolimits_{h=1}^{k-1} (1 - z^h_{ij}) + z^k_{ij} + (1 - \alpha_{ij}) - \delta^k \qquad \forall i, j \in N, k \in \mathcal{K} \tag{3.17b}$$

$$z^k_{ij} = z^k_{ji} \qquad \forall i, j \in N, k \in \mathcal{K}, \tag{3.17c}$$

where $\delta^k = \min\{|r^k_i - r^k_j| \text{ s.t. } r^k_i \neq r^k_j\}$. Note that $z^k_{ij} = 1$ in (3.17a) implies that $r^k_i = r^k_j$. Moreover, if $r^k_i = r^k_j$ and $k < k_{ij}$, then (3.17b)-(3.17c) imply that $z^k_{ij} = 0$ is infeasible. Also, note that (3.17b)-(3.17c) are trivially satisfied for $k \geq k_{ij}$ because $z^h_{ij} = 1$ for some $h < k_{ij}$.

Finally, we consider the knapsack constraints limiting item selection.

$$\sum\nolimits_{i=1}^{n} w_i x_i \leq d \tag{3.18a}$$

$$w_i \leq d - \sum\nolimits_{\substack{t=1 \\ t \neq i}}^{n} w_t q_{ti} + M(1 - x_i) \qquad \forall i \in N \tag{3.18b}$$

$$w_i + M x_i \geq d - \sum\nolimits_{\substack{t=1 \\ t \neq i}}^{n} w_t q_{ti} + \delta \qquad \forall i \in N, \tag{3.18c}$$

where M is a sufficiently large constant. Constraint (3.18a) ensures that item selection satisfies the follower's knapsack constraint. In addition, constraints (3.18b)-(3.18c) enforce item i to be selected when there is enough space left by the selection of items preferred to i. In this constraint, we have that $\delta = \min_i \{w_i - u_i\}$ and u_i is as follows:

$$u_i = \max_S \{d - \sum_{t \in S} w_t \ : \ 0 \leq d - \sum_{t \in S} w_k < w_i\} \quad \forall S \subseteq N, i \notin S.$$

As an example, if w_i is integer for all $i \in N$, then we can simply set $\delta = 1$.

The next proposition formalizes the correctness of the formulation (we omit its proof as it is embedded in the above discussion).

Proposition 21. *For any fixed* $\mathbf{y}$*,* $\mathbf{x}$ *is a greedy solution if and only if it is a feasible solution of inequalities* (3.16a)-(3.18c)*.*

From Proposition 21, **BKP** with a greedy follower admits the following single-level reformulation:

$$
\begin{aligned}
\text{[g-BKP]} \quad \min_{\mathbf{y},\mathbf{x},\alpha,\mathbf{q},\mathbf{z}} \quad & f(\mathbf{y},\mathbf{x}) := \sum_{i=1}^{n_2} \big(g_{i0} + \sum_{j=1}^{n_1} g_{ij} y_j\big) x_i + \sum_{j=1}^{n_1} t_j y_j \\
\text{subject to} \quad & (3.16a) - (3.16e), \\
& (3.17a) - (3.17c), \\
& (3.18a) - (3.18c), \\
& \alpha_{ij}, q_{ij}, z_{ij}^k, x_i \in \{0,1\} \qquad \forall i,j \in N, \ \forall k \in \mathcal{K}
\end{aligned}
$$

3.4.2.3 BKP with exact and greedy followers. From the above derivations, we conclude that if set $\mathcal{H}$ includes only greedy-like algorithmic methods, then we can reformulate **RBP** and **Γ-RBP** as a single-level MIP problem. In addition, if $\mathcal{H}$ also includes an exact method, then model (3.5) and Algorithm 1 can be exploited to find solutions for **RBP** and **Γ-RBP**.

Specifically, assume, for example, that $\mathcal{H}$ in **Γ-RBP** includes an exact (optimistic) method, h_1, and several greedy approaches, $h_2, \ldots, h_{|\mathcal{H}|}$. We define extra binary variables $\mathbf{x}^h$ for all $h \in \mathcal{H}$. To solve **Γ-RBP**, we need to add the following constraints to problem (3.5): the leader's constraint (3.12b), inequalities (3.16a)–(3.18c) for $\mathbf{x}^{h_2}, \ldots, \mathbf{x}^{h_{|\mathcal{H}|}}$, and $w^\top \mathbf{x}^{h_1} \leq d$. Because $\mathbf{x}^{h_1}$ reflects the follower's exact method, then we simply apply Algorithm 1, where in Step 1 we solve the modified problem (3.5) as a single-level relaxation of the original problem. In Step 2 the stopping criteria is evaluated to verify whether $\mathbf{x}^{h_1}$ is an exact solution of the follower's problem. Finally, in Step 3 we add cuts to ensure that the algorithm converges to the appropriate values of $\mathbf{x}^{h_1}$, i.e., an optimal follower's solution given leader's decision $\mathbf{y}$.

3.5 NUMERICAL ILLUSTRATION

In this section we illustrate the modeling framework and structural results established in Sections 3.2 and 3.3 by a series of numerical experiments.

3.5.1 Defender-Attacker Problem (DAP)

In this section we consider a class of the defender-attacker problems that can be formulated as **BKP** and apply the solution techniques described in Section 3.4. **DAP** is an important and well studied problem in bilevel optimization, see, e.g. [27], [115] and references therein. Interesting results on this class and other related classes of bilevel problems can be found in [25, 58, 98].

We consider a **DAP** variant in which a defender, as the leader, allocates defensive resources among the various facilities in a set I to reduce a total restoration cost (subject to a defense budget B), and the attacker, as the follower, selects facilities to attack. More precisely, on the upper level the defender incurs on a cost of $g_{i0} - g_i \cdot y_i$ to restore facility $i \in I$ after an attack, where g_{i0} represents the cost of restoring facility i if unprotected when attacked, g_i denotes a marginal cost reduction per unit of defensive resource, and y_i denotes the defensive resources allocated to facility $i \in I$. In addition, we denote by b_i the marginal cost of allocating a unit of defensive resource to facility i. The defender's objective is to minimize the total recovery cost.

On the lower level, for a given defensive resource allocation, the attacker selects targets among the same various facilities, so as to maximize the total damage inflicted by attacking said facilities; the damage inflicted by attacking facility $i \in I$ (as perceived by the attacker) is given by $c_{i0} - c_i y_i$, where c_{i0} denotes the base damage inflicted to an unprotected facility i, and c_i is a marginal damage reduction per unit of defensive resource. The attacker aims at maximizing the total damage inflicted, subject to a total budget on attacking resources. In this regard, we let w_i denote the amount of said resources necessary to attack facility $i \in I$, and K the overall budget on attacking resources.

Assuming a rational follower (in the sequel, we refer to the defender (attacker) and leader (follower) interchangeably), the **DAP** described above can be formulated as follows.

$$[\textbf{DAP}] \quad \min_{\mathbf{y} \in \mathbb{Y}} \quad f_1(\mathbf{y}, \mathbf{x}) := \sum_{i \in I} (g_{i0} - g_i y_i) x_i \tag{3.20a}$$

$$\text{subject to} \quad \mathbf{x} \in \mathcal{X} := \operatorname*{argmax}_{\hat{\mathbf{x}} \in \{0,1\}^{|I|}} \left\{ f_2(\mathbf{y}, \hat{\mathbf{x}}) = \sum_{i \in I} (c_{i0} - c_i y_i) \hat{x}_i \mid \sum_{i \in I} w_i \hat{x}_i \leq K \right\}, \tag{3.20b}$$

where $\mathbb{Y} := \{y \in \mathbb{R}_+^{|I|} : \; g_{i0} - g_i y_i \geq 0, \; c_{i0} - c_i y_i \geq 0 \; \forall i \in I, \; \sum_{i \in I} b_i y_i \leq B\}$ denotes the feasible region of possible defensive resource allocations, while the follower's (attacker's) decision variable, $\hat{x}_i$, is equal to 1 if and only if facility i attacked.

In our computational experiments we use randomly generated instances of **DAP** where all parameters are integers generated as follows: $g_{i0} \sim U[0, 100]$, $c_{i0} \sim U[0, 50]$, $g_i, c_i \sim U[0, 2]$, $b_i, w_i \sim U[0, 20]$ for all $i \in I$, where $U[\cdot, \cdot]$ denotes a discrete uniform distribution. Furthermore, we let $B = \sum_{i \in I} b_i$ and $K = 0.5 \sum_{i \in I} w_i$. All experiments are conducted on an Intel Xenon PC with 3.7 GHz CPU and 32 GB of RAM, and MIPs are solved using CPLEX 12.4 ([67]).

3.5.2 Results and Discussion

Note that for a given upper-level decision (i.e., a defensive resource allocation), the attacker's problem in **DAP** reduces to the standard 0-1 knapsack problem. The attacker, solves his problem either exactly or by using a greedy approach outlined in Section 3.4.2.

Specifically, in our experiments the attacker's set of alternative solution methods, $\mathcal{H}$, consists of an exact method, h_1, and two Greedy Heuristics, h_2 and h_3. Thus, $|\mathcal{H}| = 3$. We assume that for h_2 the rating functions are given by $r_i^1(c_i, w_i) = c_i$ and $r_i^2(c_i, w_i) = w_i$, while for h_3 the rating functions are $r_i^1(c_i, w_i) = c_i/w_i$ (i.e., the classical cost-to-weight ratio) and $r_i^2(c_i, w_i) = w_i$, where $i \in I$.

Exploring Γ-RBP and RBP. In this set of experiments we explore how the leader's optimal decisions both under **Γ-RBP** or **RBP** and the follower's responses affect the objective function values at both levels. Specifically, we consider three instances of **DAP** with $|I| = 15$. The results of our experiments are depicted in Figures 6(a)-(i).

The results for the first instance of **DAP** are given in Figures 6(a)-(c). Specifically, Figure 6(a) displays the leader's objective function values, f_1, when the leader implements $\mathbf{y}^*_\Gamma$, $\Gamma \in \{1, 2, 3\}$. The follower responds using methods h_1, h_2 and h_3; thus, for each $\mathbf{y}^*_\Gamma$ there are three bars in Figure 6(a), each corresponding to one of the follower's solution methods. Similarly, Figure 6(b) depicts the follower's objective function values, f_2, given his responses via one of the methods. The leader's loss values, $\Delta_h(\mathbf{y}^*_\Gamma)$, are illustrated in Figure 6(c) for $\Gamma \in \{1, 2, 3\}$ and different methods h_1, h_2 and h_3.

Recall that by the definition of **Γ-RBP**, the defender takes into account only Γ out of $|\mathcal{H}|$ possible solution methods of the attacker. Thus, for $\Gamma = 1$ in Figure 6(a), the defender takes into account only method h_2 and disregards h_1 and h_3. Consequently, as the defender's hedges only against the best possible outcome, her objective function attains the best possible value, $z_{\Gamma=1}$, if she implements $\mathbf{y}^*_{\Gamma=1}$ and the attacker responds using h_2. Note that in this case, the defender's loss, $\Delta_{h_2}(\mathbf{y}^*_{\Gamma=1})$, is equal to zero. On the other hand, if the defender's guess about the attacker's response is incorrect (i.e., the attacker's uses either h_1 or h_3) then her losses can be rather substantial, which can be observed by comparing $\Delta_{h_1}(\mathbf{y}^*_{\Gamma=1})$ and $\Delta_{h_3}(\mathbf{y}^*_{\Gamma=1})$ against $\Delta_{h_2}(\mathbf{y}^*_{\Gamma=1})$ in Figure 6(c). Also, it is quite intuitive that the attacker obtains his best possible objective function values (i.e., he inflicts the most damage to the defender) whenever the leader has an incorrect assumption about the attacker's method, see, e.g., the values of f_2 with h_1 and h_3 for $\Gamma = 1$ in Figure 6(b).

In Figure 6(a) for $\Gamma = 2$ the defender takes into account two out of three of the possible solution methods used by the attacker, which, in this instance, turn out to be h_1 and h_3. The defender's objective function value, z_Γ, increases, which is consistent with Proposition 15.

The case of $\Gamma = |\mathcal{H}| = 3$ corresponds to the most conservative defender, where **Γ-RBP** reduces to **RBP** as she hedges against all three possible solution methods used by the attacker. Clearly, as the defender hedges against all three solution methods her objective function in the worst case for $\mathbf{y}^*_{\Gamma=3}$ is better than the worst cases of $\mathbf{y}^*_{\Gamma=1}$ and $\mathbf{y}^*_{\Gamma=2}$. Note also that Corollary 8 is illustrated in Figures 6(a), as for any value of $\Gamma \in \{1, 2, 3\}$, $z^*_\Gamma \leq z^*_{\mathcal{H}} = z^*_{\Gamma=3}$.

Figure 6(c) depicts losses $\Delta_h(\mathbf{y}^*_\Gamma)$, $h \in \{h_1, h_2, h_3\}$. These losses are caused by lower-level uncertainty. Thus, we can interpret these values as the "value of information" for the defender regarding lower-level uncertainty.

Finally, the other two instances are illustrated in Figures 6(d)-6(f) and Figures 6(g)-6(i), respectively. These results are consistent with those depicted in Figures 6(a)-6(c). Recall that whenever the defender solves model **Γ-RBP**, she does not hedge against a fixed subset of the attacker's methods, but rather ensures that Γ out of them are taken into account, while $|\mathcal{H}| - \Gamma$ worst outcomes for the defender are discarded. Thus, it is worth pointing out that for the same value of $\Gamma \in \{1, 2\}$ in Figures 6(a), 6(d) and 6(g) the defender takes into account different subsets of the attacker's solution methods.

The leader's loss analysis. In this set of experiments, we provide a more detailed exploration of the defender's losses under different scenarios. In Figure 7(a) we depict the defender's loss ratio, $\Delta_h(\mathbf{y})/f^*_h$, where the attacker selects a method from h_1, h_2 or h_3 to respond to the defender's decision, $\mathbf{y}$. The latter is assumed to be computed based on one of the following six methods. In the first three, the defender assumes that the attacker always selects a specific method h and thus, she implements $\mathbf{y}^h$. In the next three, she decides based on the **Γ-RBP** model, where $\Gamma \in \{1, 2, 3\}$ and implements $\mathbf{y}^*_\Gamma$. Furthermore, Figure 7(b), depicts the defender's ex-post average loss ratio, $\Delta^{\text{A}}_{h'h}/f^*_h$, for $h, h' \in \{h_1, h_2, h_3\}$. The results for both figures are obtained for ten **DAP** instances, where $|I| = 15$ and $|\mathcal{H}| = 3$, and the average loss ratio is reported. In each figure the error bars represent the smallest and largest loss ratios.

In Figure 7(a) the first three bars, for each of the defender's solution method h_1, h_2 and h_3, represent the leader's loss ratio due to her incorrect guess about the attacker's response. If her guess is correct, then by definition, $\Delta_h(\mathbf{y}^h) = 0$ (see Definition 2), and consequently her loss ratio is zero. For example, in Figures 7(a), there is no "blue bar" for attacker's method h_1, meaning that when the defender implements $\mathbf{y}^{h_1}$ and the attacker responds based on method h_1, then the defender's loss ratio is zero. Otherwise, the defender's loss can be rather significant when her guess about the attacker's behavior is incorrect. For example, see the "blue bar" for h_2 in Figures 7(a) which represents $\Delta_{h_2}(\mathbf{y}^{h_1})/f^*_{h_2}$.

On the other hand, Figures 7(a) illustrates how employing **Γ-RBP** to hedge against all attacker's potential responses, influences the defender's loss ratio. Note that, because in $\Gamma = 1$ the defender ignores two possible responses, her loss still can be large. See, for example the "gray bar" for methods h_1 and h_3. However, her loss ratio decreases by increasing the value of Γ to $\Gamma = 2$ and $\Gamma = 3$. For example, for any attacker's method, the defender's loss ratio for $\Gamma = 3$, "green bar," is among the smallest values of loss ratios.

Finally, Figures 7(b) displays the leader's ex-post loss ratio, $\Delta^{\mathrm{A}}_{h'h}/f^*_h$, under different situations. If the attacker applies a method which is anticipated by the defender, then by definition the defender's ex-post loss value is zero (see Definition 3). Note that, defender's ex-post loss ratio can be larger than her actual loss ratio. For example, compare the "red bar" in Figures 7(b), for attacker's method h_1, with the corresponding value in Figures 7(a). In other words, even when the defender's objective functions is much smaller than she expected, in fact, her actual losses are not necessarily that substantial.

Comparing RBP, Γ-RBP and PBP. Finally, in the last set of our experiments, we compare the defender's expected loss value, see (3.8), when she applies one of the **PBP**, **Γ-RBP** (for $\Gamma = 2$) or **RBP** models, i.e., she implements as her decisions $\mathbf{y}^*_p$, $\mathbf{y}^*_{\Gamma=2}$ or $\mathbf{y}^*_{\Gamma=3}$, respectively. These experiments illustrate the effect of incorporating p_h into our framework, on reducing the defender's expected loss value. In other words, if the leader has some additional information, then she can exploit it to implement decisions that potentially reduce her expected losses. In our context, this information consists of probabilities of implementing a particular solution method by the attacker.

We use a specific instance of **DAP** in which $|I| = 15$ and $\mathcal{H} = \{h_1, h_2, h_3\}$. The parameters of the defender's problem are $\mathbf{g}_0 = [110\ 30\ 35\ 3.5\ \ldots\ 3.5\ 5\ 10]^\top$, $\mathbf{g} = [3\ 3\ 2\ \ldots\ 2\ 5]^\top$, $b_i = 1$ for all $i \in I$ and $B = 5$. In addition, for the attacker's problem we have $\mathbf{c}_0 = [15M\ 15M\ 5000\ 720\ 605\ 500\ 405\ 320\ 245\ 180\ 125\ 80\ 45\ 20\ 0]$, $\mathbf{c} = [0\ 0\ 0\ 12\ 11\ 10\ 9\ 8\ 7\ 6\ 5\ 4\ 3\ 2\ 0]^\top$, $\mathbf{w} = [M\ \ M+1\ 5000\ 60\ 55\ 50\ 45\ 40\ 35\ 30\ 25\ 20\ 15\ 10\ 5]^\top$ and $K = M + 5001$, where M is a sufficiently large constant. The defender's optimal solutions for different attacker's responses is presented in Table 3.

Table 3: Leader's optimal solution and her corresponding objective function value for follower's different solution methods for the **DAP** instance used in Figure 8

h	$\mathbf{y}^h$	f_h^*
h_1	$\mathbf{y}^{h_1} = (0\ 5\ 0\ \ldots\ 0)^\top$	50
h_2	$\mathbf{y}^{h_2} = (5\ 0\ \ldots\ 0)^\top$	130
h_3	$\mathbf{y}^{h_3} = (0\ \ldots\ 0\ 5)^\top$	135

The defender's expected loss value, $\mathbb{E}_h[\Delta_h(\mathbf{y})]$, is illustrated in Figures 8(a)-(f) as a function of p_h, $h \in \{h_1, h_2, h_3\}$, where we fix the value of p_h for a specific method in each figure. For a fixed defender's decision $\mathbf{y}$, the value of $f(\mathbf{y}, \mathbf{x}^h(\mathbf{y}))$ can be computed for any method $h \in \mathcal{H}$, and then $\mathbb{E}_h[\Delta_h(\mathbf{y})]$ is a linear function of p_h, see equation (3.8). Note that for **Γ-RBP** and **RBP**, the defender's decisions do not depend on the information available to **PBP**, i.e., the probability distributions. Thus, given decisions $\mathbf{y}^*_{\Gamma=2}$ and $\mathbf{y}^*_{\Gamma=3}$, in **Γ-RBP** and **RBP**, the defender's expected losses are linear function of p_h, which can be observed in Figures 8(a)-(f).

On the other hand, for the **PBP** model the defender incorporates this additional information into her decision making, and thus, the value of $\mathbf{y}^*_p$ changes for different values of p_h, $h \in \mathcal{H}$. Consequently, $\mathbb{E}_h[\Delta_h(\mathbf{y})]$ is a piece-wise linear function of p_h in **PBP**, see Figures 8(a)-(f).

Furthermore, compared to **Γ-RBP**, model **PBP** always results in smaller values of expected losses. This observation is not surprising, given that the defender's objective function in **PBP** is equivalent to minimizing the expected loss value, see (3.8). This reduction in the expected losses can be interpreted as the value of additional information available to the defender.

Recall that for **Γ-RBP**, only Γ methods out $|\mathcal{H}|$ are taken into account by the defender. In Figure 8, for the **Γ-RBP** model, we set $\Gamma = 2$, and thus, one of the attacker's solution methods is disregarded by the defender. Consequently, whenever the probability of implementing this method is sufficiently high (small), the expected losses of **RBP** are smaller (higher) than those of **Γ-RBP**.

For example, in Figure 8(c), **Γ-RBP** hedges against h_1 and h_2, while h_3 is disregarded. The value of $p_{h_1} = 0$ in Figure 8(c). Thus, when the value of p_{h_2} is sufficiently small, $0 \leq p_{h_2} \leq 0.4$, the corresponding probability of implementing h_3 is rather high. Consequently, the expected losses of **Γ-RBP** are worse than those of both the **RBP** and **PBP** models. On the other hand, as the value of p_{h_2} increases, given that $p_{h_1} = 0$, the value of p_{h_3} decreases resulting in better and worse expected losses for **Γ-RBP** and **RBP**, respectively.

3.6 CONCLUSION

One of the key assumptions in the standard bilevel optimization modeling framework is that the follower solves his problem optimally. However, there are many practical application settings where this assumption is not likely to hold. In this chapter, we propose an approach for addressing this issue. By assuming that a set of possible follower's solution methods is known, we propose three modeling approaches, namely, **RBP**, **Γ-RBP** and **PBP**, that allow the leader to hedge against different response scenarios at the lower level, which we refer to as the lower-level algorithmic uncertainty.

Among the proposed approaches, the **RBP** model is the most conservative one as it hedges against all possible follower's solution methods. On the other hand, the **Γ-RBP** model allows the leader to control the level of her conservatism through a fixed parameter Γ.

Finally, the **PBP** model assumes that some additional probabilistic information is available to the leader, who exploits it in the decision-making process.

We explore theoretical properties of the proposed models, and illustrate its application using a broad class of the bilevel knapsack problems in the context of the defender-attacker model. Our results indicate that the proposed approaches allow the leader to substantially reduce her losses whenever the follower's actual behavior is not known precisely.

With respect to the future research directions, it would be valuable to derive additional single-level reformulations of bilevel problems with irrational followers where the lower-level algorithmic uncertainty extends beyond the use of greedy heuristics. Another interesting direction includes settings where the leader and the follower interact repeatedly over time, and hence the leader might infer information regarding the method used by the follower based on his response to the leader decisions.

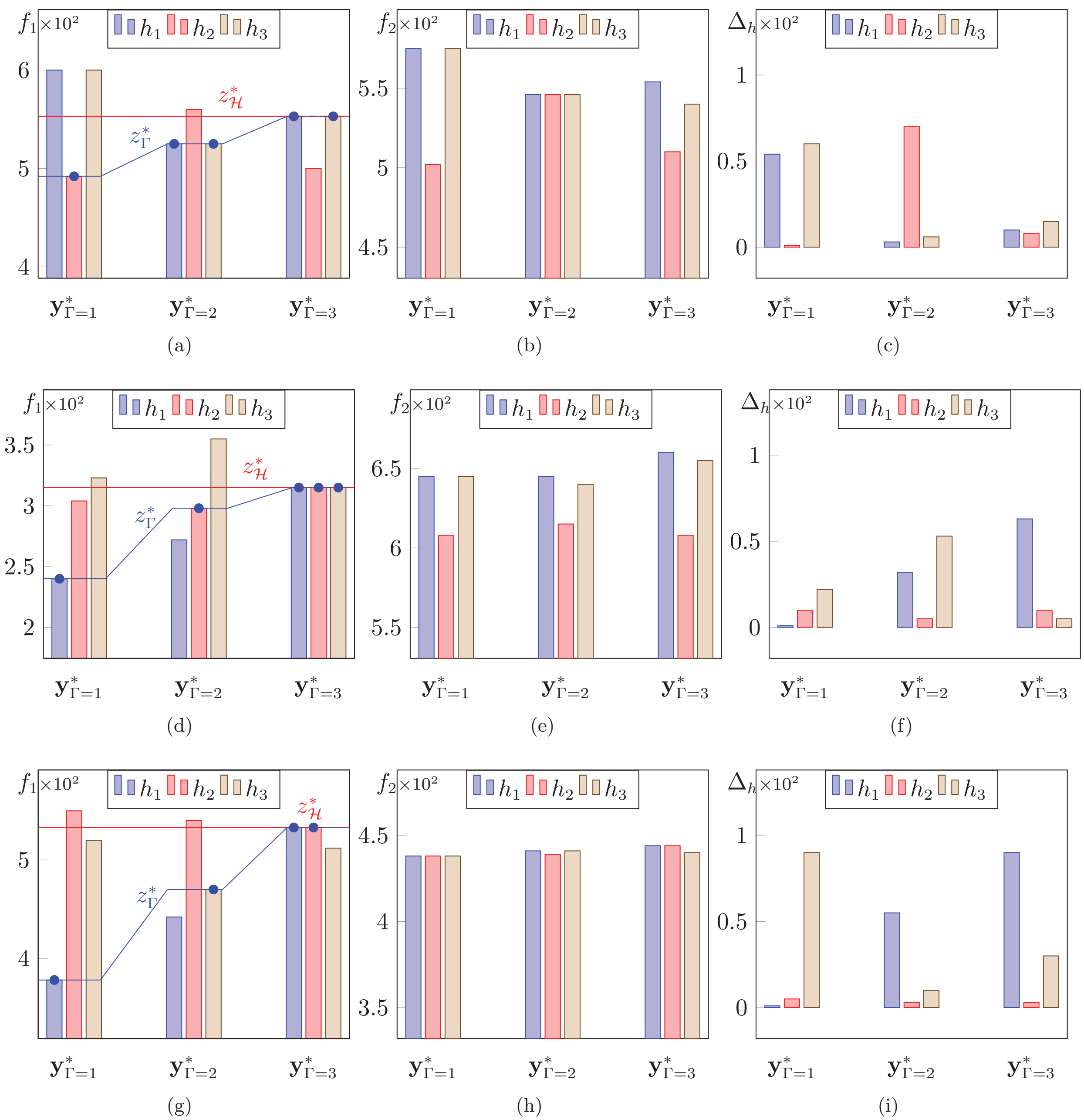


Figure 6: Illustration of Proposition 15 and Corollary 8 for three **DAP** instances where $|I| = 15$ and $|\mathcal{H}| = 3$. The results for the first instance are given in Figures 6(a)-(c). Specifically, the defender implements $\mathbf{y}^*_\Gamma$, $\Gamma \in \{1, 2, 3\}$, and the attacker responds using methods h_1, h_2 and h_3. Figures 6(a) and 6(b) depict the defender's and the attacker's objective function values, f_1 and f_2, respectively, for each follower's method (thus, three different bars) given leader's decision $\mathbf{y}^*_\Gamma$, $\Gamma \in \{1, 2, 3\}$. The leader's loss values, $\Delta_h(\mathbf{y}^*_\Gamma)$, are illustrated in Figure 6(c) for $\Gamma \in \{1, 2, 3\}$ and different methods h. The value of z^*_Γ for $\Gamma \in \{1, 2, 3\}$ is shown in Figure 6(a). Figures 6(d)-6(f) and Figures 6(g)-6(i) display the same information for two additional instances of **DAP**.

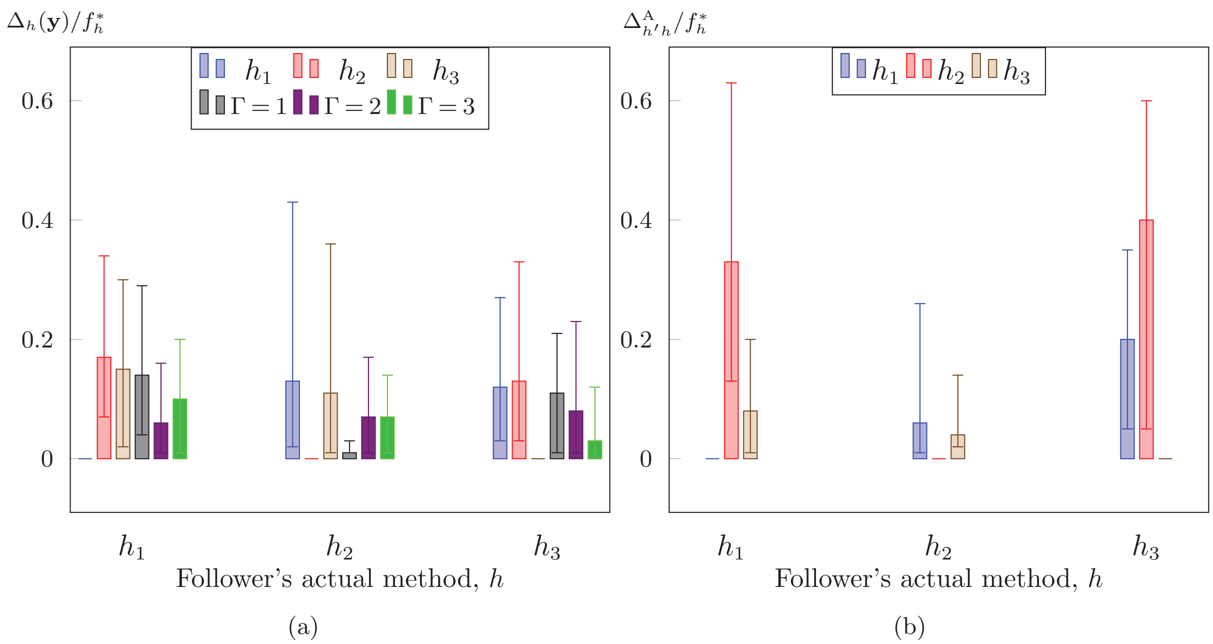
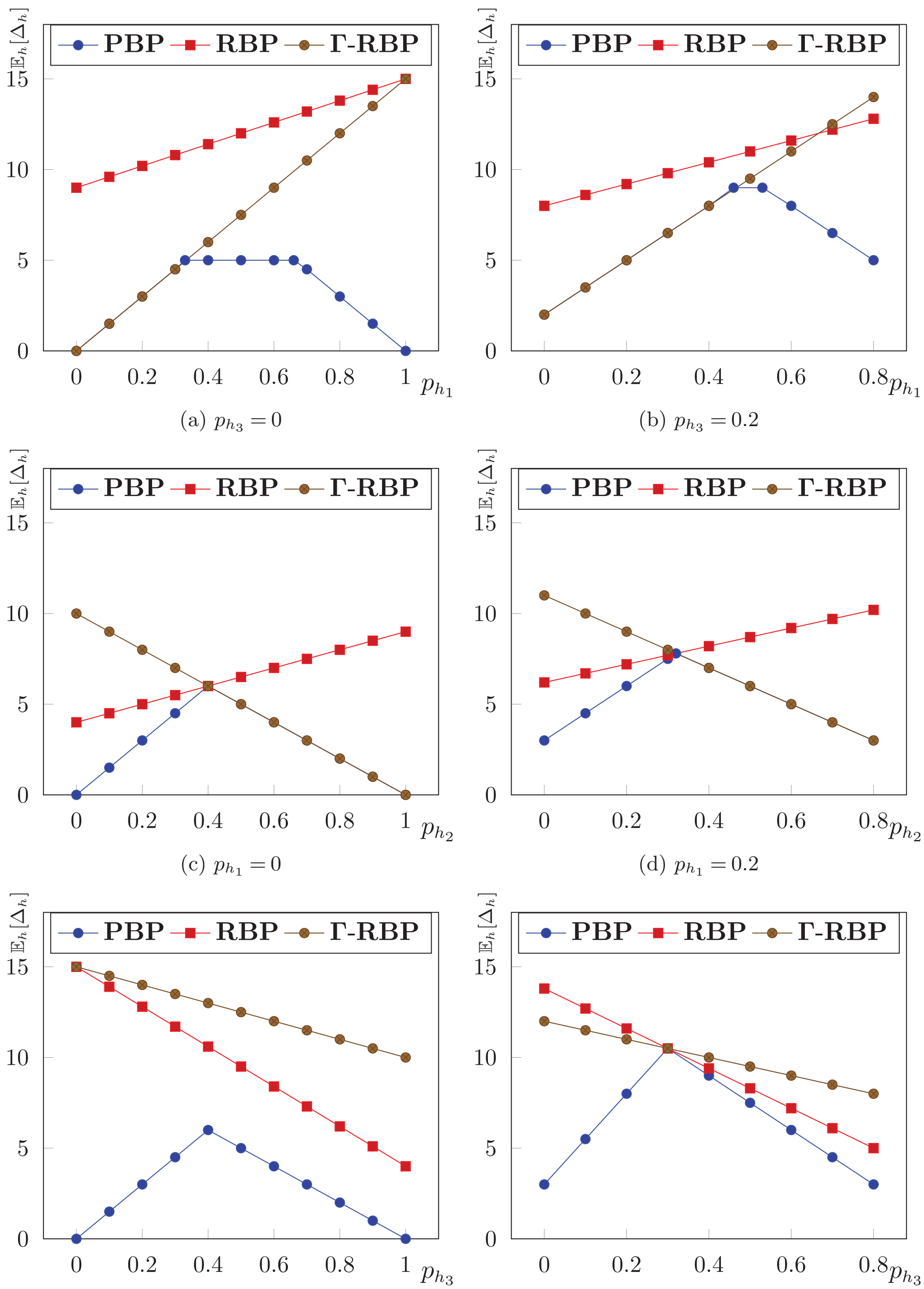


Figure 7: Illustration of the (defender's) loss ratios, $\Delta_h(\mathbf{y})/f_h^*$ and $\Delta^{\mathrm{A}}_{h'h}/f_h^*$, under different situations. The defender's loss is considered for each possible solution method of the attacker, i.e., h_1, h_2 and h_3. In (a) for each attacker's solution approach, the defender's decision, $\mathbf{y}$, is assumed to be computed based on one of the following six methods (depicted in different colors). In the first three, the defender assumes that the attacker always selects a specific method h and thus, she implements $\mathbf{y}^h$. In the next three, she decides based on the (γ, α)-**BMIP** model, where $\Gamma \in \{1, 2, 3\}$ and thus, she implements $\mathbf{y}^*_\Gamma$. In (b) we depict the defender's ex-post average loss ratio $\Delta^{\mathrm{A}}_{h'h}/f_h^*$ (relative to her expectations). The results are obtained for ten **DAP** instances where $|I| = 15$ and $|\mathcal{H}| = 3$. The error bars represent the smallest and largest loss ratios.



(a) $p_{h_3} = 0$ (b) $p_{h_3} = 0.2$

(c) $p_{h_1} = 0$ (d) $p_{h_1} = 0.2$

(e) $p_{h_2} = 0$ (f) $p_{h_2} = 0.2$

Figure 8: Illustration of the defender's expected loss value as a function of p_h, $h \in \mathcal{H}$ for a **DAP** instance with $|I| = 15$ and $|\mathcal{H}| = 3$. For **Γ-RBP**, $\Gamma = 2$. Thus, the expected losses values are displayed for defender's decision $\mathbf{y}_p^*$, $\mathbf{y}_{\Gamma=2}^*$ and $\mathbf{y}_{\Gamma=3}^*$, i.e., when she uses **PBP**, **Γ-RBP** and **RBP**, respectively. In each figure, p_h is fixed for a specific method h and the defender's expected loss values for different approaches are compared.

4.0 ON LINEARIZED REFORMULATIONS FOR A CLASS OF BILEVEL LINEAR INTEGER PROBLEMS

4.1 INTRODUCTION

In this chapter we consider a class of bilevel linear integer problems (BLIPs) where the leader's and follower's objective functions and constraints are affine functions of the decision variables. Such bilevel problems encompass many applications across different fields, including economics, energy, defense, pricing, among others, see [38, 41, 81] and the references therein. Formally, we focus on BLIPs of the form:

$$\zeta^* = \max_{x,y} \big\{ \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \ : \ x \in X, \ y \in \operatorname*{argmax}_{\hat{y}} \{ \boldsymbol{c}^\top \hat{y} \ : \ \hat{y} \in Y(x) \} \big\}, \tag{4.1}$$

where $X = \{x \in \mathbb{Z}^q_+ \ : \ \boldsymbol{H}x \leq \boldsymbol{h}\}$ and $Y(x) = \{y \in \mathbb{R}^n_+ \ : \ \boldsymbol{F}y + \boldsymbol{L}x \leq \boldsymbol{f}\}$ denote the leader's and the follower's feasible sets, respectively, with $\boldsymbol{a} \in \mathbb{R}^q$, $\boldsymbol{d} \in \mathbb{R}^n$, $\boldsymbol{H} \in \mathbb{R}^{p\times q}$, $\boldsymbol{h} \in \mathbb{R}^p$, $\boldsymbol{F} \in \mathbb{R}^{m\times n}$, $\boldsymbol{L} \in \mathbb{R}^{m\times q}$ and $\boldsymbol{f} \in \mathbb{R}^m$. BLIPs given by (4.1) are clearly NP-hard as linear mixed-integer problems form a special class of (4.1). Furthermore, bilevel linear problems (BLPs) obtained by relaxing the integrality restrictions in X are also known to be NP-hard [61, 71]. Bilevel problems that involve integrality restrictions at the lower level [45, 104] are outside the scope of this note.

Arguably, the most common methods of solving bilevel problems are based on reformulating them as single-level problems by replacing a linear problem (LP) at the lower level by its optimality conditions, e.g., Karush-Kuhn-Tucker (KKT) optimality conditions. From this single-level reformulation, BLPs and BLIPs of form (4.1) can be further reformulated as linear mixed-integer problems (linear MIPs), see, e.g., [9, 10, 48]. From the implementation perspective, such linear MIP reformulations have important advantages, as they provide the opportunity for application of off-the-shelf MIP solvers. Unfortunately, the typical KKT-based MIP reformulation introduces a new binary variable for each complementary slackness condition at the lower level, and as a consequence, might not be scalable for many practical instances of bilevel problems.

To address this drawback, in this note we explore MIP reformulations of BLIPs that exploit the strong duality (SD) property of LPs. Simply speaking, this approach replaces the complementarity slackness constraints that result from the KKT conditions, by a single quadratic constraint derived from the strong duality property. Under the assumption that the upper-level variables are integer, this quadratic constraint can be linearized by considering the binary decomposition of the integer variables and applying classical 0–1 linearization approaches (see e.g., [56, 57, 79, 109]).

Specifically, in this note we describe two alternative linearization methods of the strong duality constraint. In contrast to the KKT-based counterpart, the number of required new binary variables in SD-based reformulations is independent from the number of lower-level variables and constraints. Particularly, if the upper-level variables are restricted to be binary, then the reformulations do not introduce new discrete variables. In a more general setting, where the upper-level variables are integer, these reformulations introduce $O(q \log(U))$ new binary variables, where q is the number of upper-level variables and U is a valid upper bound for all upper-level variables. However, the introduction of fewer binary variables in the SD-based reformulations comes at the price of introducing more continuous variables, and potentially, more linear constraints.

To the best of our knowledge the considered SD-based linearized models of (4.1) are new except one of them for the case of binary variables, see further details and references in subsection **R2** of Section 4.2. As mentioned earlier we describe two alternative ways of linearizing the strong duality constraint, and each of them can handle both general integer and binary cases. It should be noted that the discussed reformulations are fairly straightforward and are based on combinations of two classical ideas from the MIP literature, namely, (i) the linearization approach of a product of two variables given that at least one of them is binary and (ii) the binary representation that uses a logarithmic number of variables in terms of the problem's primitives. In particular, the former idea is a building block for linearized models of many nonlinear (e.g., quadratic and fractional) binary problems, see [3, 56, 57, 102, 109, 112] and the references therein. Detailed discussions of the latter idea can be found in [4, 107]. Approaches based on their combinations have also been used for linearizing fractional 0–1 and mixed integer bilinear problems [24, 59].

Finally, we are not aware of any systematic studies that perform the computational comparisons between KKT- and SD-based reformulations of BLIPs. More importantly, in our experiments we observe that for many test instances the SD-based reformulations are orders of magnitude faster than KKT-based one. This speed-up is more noticeable for BLIPs that involve a lower-level problem with sufficiently more variables and constraints than the upper-level problem, which is intuitive given the sizes of the obtained linearized models. We believe that this observation is an important contribution to the bilevel optimization literature.

4.2 MIP REFORMULATIONS

In this section we consider BLIPs given by (4.1), where it is assumed that set X is nonempty and bounded and for any leader's solution $x \in X$, set $Y(x)$ is also nonempty and bounded. Therefore, there exists an optimal solution of (4.1). Furthermore, we also assume that the bilevel model (4.1) follows the *optimistic* approach, which implies that when facing with multiple lower-level optimal solutions, the follower picks the one that favors the leader most, i.e., the leader and follower are cooperative. All of the above assumptions are standard in the bilevel optimization literature [38].

Next, we present three possible linear MIP reformulations of (4.1) and compare their sizes in terms of the number of variables (both continuous and discrete) and the number of constraints. We note that without any additional assumptions, these reformulations are not comparable in terms of their LP relaxation quality. That is, in general no reformulation is better than the others in terms of their LP relaxation quality. Particularly, as shown in our experiments in Section 4.3, there are different relationships between the quality of the relaxations that depend on the structure and the data of the bilevel problem.

Reformulation 1 (R1). The first reformulation referred to as **R1**, replaces the lower-level problem by its optimality conditions and then linearizes the resulting optimization problem by applying the big-M method. This approach is the most common in the bilevel optimization literature and has been studied in a number of papers, see, e.g., [9, 10, 13, 14, 23, 29, 48, 72, 117].

Specifically, replacing the lower-level problem in (4.1) by its KKT conditions yields a single-level nonlinear problem given by:

$$\zeta^* = \max_{x,y,\theta} \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.2a}$$

$$\text{subject to} \quad \boldsymbol{H}x \leq \boldsymbol{h} \tag{4.2b}$$

$$\boldsymbol{F}y + \boldsymbol{L}x \leq \boldsymbol{f} \tag{4.2c}$$

$$-\boldsymbol{F}^\top \theta \leq -\boldsymbol{c} \tag{4.2d}$$

$$(\boldsymbol{f} - \boldsymbol{F}y - \boldsymbol{L}x)^\top \theta = 0 \tag{4.2e}$$

$$(\boldsymbol{F}^\top \theta - \boldsymbol{c})^\top y = 0 \tag{4.2f}$$

$$x \in \mathbb{Z}_+^q, \ y \in \mathbb{R}_+^n, \ \theta \in \mathbb{R}_+^m. \tag{4.2g}$$

In the problem (4.2a)–(4.2g), the dual variables of the lower-level LP are denoted by $\theta_1, \ldots, \theta_m$, where its primal and dual feasibility constraints are given by (4.2c) and (4.2d), respectively. The complementary slackness constraints of the lower-level problem are given by equations (4.2e) and (4.2f). Therefore, a point $(y, \theta) \in \mathbb{R}_+^n \times \mathbb{R}_+^m$ satisfies the equations (4.2c)-(4.2f) if and only if it satisfies the KKT optimality conditions of the lower-level problem given the leader's decision x.

Let (x^*, y^*, θ^*) be an optimal solution of (4.2). Let M and $\widetilde{M}$ be sufficiently large constants such that $M \geq \max\{\|\boldsymbol{f} - \boldsymbol{F}y^* - \boldsymbol{L}x^*\|_\infty, \ \|\theta^*\|_\infty\}$ and $\widetilde{M} \geq \max\{\|\boldsymbol{F}^\top \theta^* - \boldsymbol{c}\|_\infty, \ \|y^*\|_\infty\}$, where $\|\boldsymbol{b}\|_\infty = \max_{i=1,\ldots,\ell}\{b_i\}$ for any vector $\boldsymbol{b} \in \mathbb{R}^\ell$. Then, by introducing new binary variables $u \in \{0,1\}^m$ and $v \in \{0,1\}^n$, nonlinear constraints (4.2e) and (4.2f) can be linearized, which implies that problem (4.2) is equivalent to:

$$(\mathbf{R1}) \quad \zeta^* = \max_{x,y,\theta,u,v} \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.3a}$$

$$\text{subject to} \quad (4.2b) - (4.2d) \tag{4.3b}$$

$$\boldsymbol{f} - \boldsymbol{F}y - \boldsymbol{L}x \leq Mu \tag{4.3c}$$

$$\theta \leq M(\mathbf{1} - u) \tag{4.3d}$$

$$\boldsymbol{F}^\top \theta - \boldsymbol{c} \leq \widetilde{M} v \tag{4.3e}$$

$$y \leq \widetilde{M}(\mathbf{1} - v) \tag{4.3f}$$

$$x \in \mathbb{Z}_+^q,\ y \in \mathbb{R}_+^n,\ \theta \in \mathbb{R}_+^m \tag{4.3g}$$

$$u \in \{0,1\}^m,\ v \in \{0,1\}^n, \tag{4.3h}$$

where $\mathbf{1}$ denotes vectors of all ones of appropriate dimensions. Constraints (4.3c)-(4.3d) and constraints (4.3e)-(4.3f) are the linearized versions of the nonlinear constraints (4.2e) and (4.2f), respectively. Because u is a binary variable, the right-hand side in either of inequalities (4.3c) or (4.3d) is zero and thus, equation (4.2e) holds. By the same arguments, it follows that the constraints (4.3e)-(4.3f) are equivalent to constraint (4.2f).

The main advantage of this MIP reformulation is that it is valid even if the upper-level variables are allowed to take continuous values, i.e., the integrality restrictions in X are relaxed. However, it assigns a new binary variable to each constraint and variable in the lower-level problem.

Reformulation 2 (R2). We can also apply the strong duality property of LPs to replace the lower-level problem and achieve a single-level problem. To the best of our knowledge, this technique has been used only for some specific classes of bilevel problems where the upper-level decision variables are required to be binary, or where the structure of the problem allows for simple linearizations of the product of certain decision variables, see [6, 7, 16, 19, 52, 53, 82–84, 87, 88, 91, 93, 97, 113]. However, this approach can be used to develop a single-level reformulation, even if the upper-level variables are general integers. For more details on these types of linearizations we refer the reader to [3] and the references therein.

In the specific bilevel problem presented in (4.1), the strong duality property results in $\boldsymbol{c}^\top y = (\boldsymbol{f} - \boldsymbol{L}x)^\top \theta$, which involves the product of variables x and θ through the expression $x^\top \boldsymbol{L}^\top \theta$. Accordingly, problem (4.1) is equivalent to the following reformulation:

$$\zeta^* = \max_{x,y,\theta} \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.4a}$$

$$\text{subject to} \quad (4.2b) - (4.2d) \tag{4.4b}$$

$$\boldsymbol{c}^\top y = (\boldsymbol{f} - \boldsymbol{L}x)^\top \theta \tag{4.4c}$$

$$x \in \mathbb{Z}^q_+, y \in \mathbb{R}^n_+, \theta \in \mathbb{R}^m_+, \tag{4.4d}$$

which includes nonlinear constraint (4.4c). In such situations, the binary expansion of the integer variables x_i, $i \in I = \{1, 2, \ldots, q\}$, can be employed to obtain a linear MIP [49, 59, 109]. Let U_i be an upper bound on the value of x_i, $i \in I$, then x_i can be written as

$$x_i = \sum_{r \in R_i} 2^{r-1} z_{ir}, \tag{4.5}$$

where $R_i = \{1, 2, \cdots, \lfloor \log_2(U_i) \rfloor + 1\}$ for all $i \in I$, and $z_{ir} \in \{0, 1\}$ for all $r \in R_i$, $i \in I$. Hence, the nonlinear term in constraint (4.4c) can be rewritten as

$$x^\top \boldsymbol{L}^\top \theta = \sum_{k \in K} \sum_{i \in I} x_i L_{ki} \theta_k = \sum_{k \in K} \sum_{i \in I} \sum_{r \in R_i} 2^{r-1} L_{ki} z_{ir} \theta_k, \tag{4.6}$$

where $K = \{1, \ldots, m\}$.

For any $i \in I$, $r \in R_i$ and $k \in K$, define $v_{irk} = z_{ir}\theta_k$. Note that v_{irk} is a continuous variable and we have $v_{irk} = \theta_k$ if $z_{ir} = 1$ and $v_{irk} = 0$, otherwise. The variables v_{irk} can replace the products $z_{ir}\theta_k$ in equation (4.6), while the constraints $v_{irk} = z_{ir}\theta_k$ can be enforced through the following linear inequalities [3, 57, 79, 109]:

$$v_{irk} \leq \theta^U_k z_{ir} \qquad \forall i \in I, r \in R_i, k \in K \tag{4.7a}$$

$$v_{irk} \leq \theta_k + \theta^L_k z_{ir} - \theta^L_k \qquad \forall i \in I, r \in R_i, k \in K \tag{4.7b}$$

$$v_{irk} \geq \theta^L_k z_{ir} \qquad \forall i \in I, r \in R_i, k \in K \tag{4.7c}$$

$$v_{irk} \geq \theta_k + \theta^U_k z_{ir} - \theta^U_k \qquad \forall i \in I, r \in R_i, k \in K, \tag{4.7d}$$

where θ^U_k and θ^L_k are upper and lower bounds, respectively, on θ_k for any $k \in K$. For any $i \in I$ and $r \in R_i$, constraints (4.7a) and (4.7c) enforce that if $z_{ir} = 0$, then $v_{irk} = 0$ for all $k \in K$; otherwise, constraints (4.7b) and (4.7d) ensure that $v_{irk} = \theta_k$ for all $k \in K$. Because θ_k is a nonnegative variable for all $k \in K$, we can also replace θ^L_k by zero and consequently remove constraint (4.7c). Therefore, problem (4.1) can be reformulated as follows:

$$(\mathbf{R2}) \quad \zeta^* = \max_{x,y,\theta,z,v} \; \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.8a}$$

$$\text{subject to} \quad (4.2b) - (4.2d) \tag{4.8b}$$

$$(4.7a) - (4.7d) \tag{4.8c}$$

$$x_i = \sum_{r \in R_i} 2^{r-1} z_{ir} \qquad \forall i \in I \tag{4.8d}$$

$$\boldsymbol{c}^\top y + \sum_{k \in K} \sum_{i \in I} \sum_{r \in R_i} 2^{r-1} L_{ki} v_{irk} = \boldsymbol{f}^\top \theta \tag{4.8e}$$

$$x \in \mathbb{Z}_+^q, \; y \in \mathbb{R}_+^n, \; \theta \in \mathbb{R}_+^m \tag{4.8f}$$

$$z_i \in \{0,1\}^{|R_i|}, \; v_i \in \mathbb{R}^{|R_i| \times m} \qquad \forall i \in I, \tag{4.8g}$$

which is the desired reformulation. In contrast with Reformulation **R1**, the number of new binary variables in **R2** does not depend on the size of the follower's linear problem but only on the number of leader's variables and their upper bounds. Furthermore, if the leader's variables in X are binary, then this approach does not introduce new binary variables. However, this reformulation is not valid if there are no integrality restrictions for the upper-level variables.

Reformulation 3 (R3). This reformulation presents an alternative approach to linearize equation (4.6) and to the best of our knowledge it has not been used before in the bilevel optimization literature. By linearizing the products between the upper-level binary decomposition variables and a linear combination of the lower-level dual variables, this method results in a significant reduction in the number of additional variables and constraints. Note that equation (4.6) can be rewritten as follows:

$$x^\top \boldsymbol{L}^\top \theta = \sum_{i \in I} \sum_{r \in R_i} 2^{r-1} z_{ir} \sum_{k \in K} L_{ki} \theta_k. \tag{4.9}$$

For any $i \in I$ and $r \in R_i$ we define a continuous variable $v_{ir} = z_{ir} \sum_{k \in K} L_{ki} \theta_k$. Therefore, in the new reformulation the linearization constraints (4.7a)-(4.7a) become the following inequalities, see [3, 56]:

$$v_{ir} \leq \Theta_i^U z_{ir} \qquad i \in I, r \in R_i \tag{4.10a}$$

$$v_{ir} \leq \left(\sum_{k \in K} L_{ki} \theta_k \right) + \Theta_i^L z_{ir} - \Theta_i^L \qquad i \in I, r \in R_i \tag{4.10b}$$

$$v_{ir} \geq \Theta_i^L z_{ir} \qquad i \in I, r \in R_i \tag{4.10c}$$

$$v_{ir} \geq \left(\sum_{k \in K} L_{ki}\theta_k\right) + \Theta_i^U z_{ir} - \Theta_i^U \qquad i \in I, r \in R_i \tag{4.10d}$$

where Θ_i^L and Θ_i^U are lower and upper bounds, respectively, on the value of $\sum_{k \in K} L_{ki}\theta_k$. The idea behind (4.9) and inequalities (4.10a)-(4.10d) is similar to that of inequalities (4.7a)-(4.7d), see further discussions in [3, 56]. For any $i \in I$ and $r \in R_i$, the constraints (4.10a) and (4.10c) ensure that if $z_{ir} = 0$ then $v_{ir} = 0$; otherwise, if $z_{ir} = 1$, then the constraints (4.10b) and (4.10d) enforce that $v_{ir} = \theta_k$.

Therefore, problem (4.1) can be written as follows:

$$(\mathbf{R3}) \quad \zeta^* = \max_{x,y,\theta,z,v} \; \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.11a}$$

$$\text{subject to} \quad (4.2b) - (4.2d) \tag{4.11b}$$

$$(4.10a) - (4.10d) \tag{4.11c}$$

$$x_i = \sum_{r \in R_i} 2^{r-1} z_{ir} \qquad \forall i \in I \tag{4.11d}$$

$$\boldsymbol{c}^\top y + \sum_{i \in I} \sum_{r \in R_i} 2^{r-1} v_{ir} = \boldsymbol{f}^\top \theta \tag{4.11e}$$

$$x \in \mathbb{Z}_+^q, \; y \in \mathbb{R}_+^n, \; \theta \in \mathbb{R}_+^m \tag{4.11f}$$

$$z_i \in \{0,1\}^{|R_i|}, \; v_i \in \mathbb{R}^{|R_i|} \quad \forall i \in I. \tag{4.11g}$$

As mentioned at the beginning of the section, the relaxation quality of the reformulations are not comparable (see also Section 3). However, under certain stringent conditions on the data and the value of the big-M constants, we have the following relationship between **R2** and **R3**.

Proposition 22. *Suppose that $L_{ki} \geq 0$ for all $k \in K$ and $i \in I$. If $\Theta_i^U \geq \sum_{k \in K} L_{ki}\theta_k^U$ and $\Theta_i^L \leq \sum_{k \in K} L_{ki}\theta_k^L$ for all $i \in I$, then* **R2** *is at least as strong as* **R3** *in terms of its LP relaxation quality.*

Proof. Let $\hat{x}$, $\hat{y}$, $\hat{\theta}$, $\hat{z}$ and $\hat{v}$ be a feasible solution in the LP relaxation of **R2**. We claim there exist x, y, θ, z, v feasible in the relaxation of **R3** that attain the same objective function value. Set $x = \hat{x}$, $y = \hat{y}$, $\theta = \hat{\theta}$, $z = \hat{z}$ and for any i, r, set $v_{ir} = \sum_{k \in K} L_{ki}\hat{v}_{ikr}$. Then it can be readily verified that x, y, θ, z, v are feasible for the LP relaxation of **R3** since $\boldsymbol{L} \geq 0$,

$\Theta_i^U \geq \sum_{k\in K} L_{ki}\theta_k^U$ and $\Theta_i^L \leq \sum_{k\in K} L_{ki}\theta_k^L$ for all $i \in I$. Moreover, this point attains the same objective function value as $\hat{x}$, $\hat{y}$, $\hat{\theta}$, $\hat{z}$ and $\hat{v}$ do in **R2**. ∎

Sizes of the Reformulations. We compare the sizes of reformulations **R1**-**R3** in terms of the numbers of discrete and continuous variables as well as the number of constraints. This information is provided in Table 4 for $x \in \mathbb{Z}_+^q$ and $x \in \{0,1\}^q$ where $\bar{R} = \sum_{i\in I}\lfloor \log_2(U_i)\rfloor + q$. Note that when the upper-level decision variables are enforced to be binary, then there is no need to use the binary representation and this reduces the number of constraints and variables in **R2** and **R3**.

Table 4: The sizes of the proposed reformulations, where p/q and m/n represent the numbers of leader's and follower's constraints/variables, respectively. Parameter $\bar{R}$ is equal to $\sum_i \lfloor \log_2(U_i)\rfloor + q$, where U_i is a valid upper bound for the value of x_i.

	Formulation	# Continuous variables	# Discrete variables	# Linear constraints
$x \in \mathbb{Z}_+^q$	**R1**	$n+m$	$q+n+m$	$p+3m+3n$
	R2	$n+m+m\bar{R}$	$q+\bar{R}$	$p+m+n+4m\bar{R}+q+1$
	R3	$n+m+\bar{R}$	$q+\bar{R}$	$p+m+n+4\bar{R}+q+1$
$x \in \{0,1\}^q$	**R1**	$n+m$	$q+n+m$	$p+3m+3n$
	R2	$n+m+mq$	q	$p+m+n+4mq+1$
	R3	$n+m+q$	q	$p+m+n+4q+1$

4.3 COMPUTATIONAL EXPERIMENTS

In this section we describe our computational experiments aimed at exploring the numerical performance of the reformulations from Section 4.2. Specifically, we reformulate three different classes of bilevel problems as single-level MIPs according to **R1**-**R3** and then solve them with CPLEX 12.4 [67]. All experiments are performed on the same machine, i.e., an Intel Xenon PC with 3.7 GHz CPU and 32 GB of RAM.

For each instance size of each problem, we generate ten test instances and report the average running time of the solver (in the column denoted by "Time") along with the LP relaxation quality (in the column denoted by "LP Qual"), see Tables 6-9, 11, 12, 15 and 16. The LP relaxation quality is given by ζ^*_{LP}/ζ^*, where ζ^*_{LP} denotes the optimal objective function value of the LP relaxation. For each test class we also report the sizes of their MIP reformulations, see Tables 5, 10 and 13. The time limit is set to 10800 seconds (3 hours).

4.3.1 Bounded Bilevel Linear Integer Problem (BBLIP)

The first considered problem contains explicit bounds on the values of the lower-level variables:

$$[\textbf{BBLIP}] \max_{x \in \mathbb{X}} \quad \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.12a}$$

$$\text{subject to} \quad \boldsymbol{H}x \leq \boldsymbol{h} \tag{4.12b}$$

$$y \in \underset{\hat{y} \in \mathbb{R}^n_+}{\operatorname{argmax}} \{\boldsymbol{c}^\top \hat{y} \ : \tilde{\boldsymbol{F}}\hat{y} + \tilde{\boldsymbol{L}}x \leq \tilde{\boldsymbol{f}}, \ \boldsymbol{I}\hat{y} \leq \boldsymbol{1}\}, \tag{4.12c}$$

where $\boldsymbol{H} \in \mathbb{R}^{p \times q}$, $\tilde{\boldsymbol{L}} \in \mathbb{R}^{\tilde{m} \times q}$, $\tilde{\boldsymbol{F}} \in \mathbb{R}^{\tilde{m} \times n}$ and $\boldsymbol{I}$ is an $n \times n$ identity matrix. In (4.12) we consider both binary and integer settings, where $\mathbb{X} = \{0,1\}^q$ or $\mathbb{X} = \mathbb{Z}^q_+$, respectively. Observe that **BBLIP** can be framed in terms of problem (4.1) by setting $\boldsymbol{F} = \left[\begin{smallmatrix} \tilde{\boldsymbol{F}} \\ \boldsymbol{I} \end{smallmatrix}\right]$, $\boldsymbol{L} = \left[\begin{smallmatrix} \tilde{\boldsymbol{L}} \\ \boldsymbol{O} \end{smallmatrix}\right]$, and $\boldsymbol{f} = \left[\begin{smallmatrix} \tilde{\boldsymbol{f}} \\ \boldsymbol{1} \end{smallmatrix}\right]$, where $\boldsymbol{O}$ is an $n \times q$ matrix of zeros. Thus, in this case $m = \tilde{m} + n$. In Table 5 we show the reformulation sizes for both integer and binary cases.

The coefficients for all matrices and vectors in (4.12) are randomly generated from a uniform distribution $U[1, 100]$. Thus, all their entries are non-zero. For any leader's constraint ℓ, $\ell \in \{1, \ldots, p\}$, we have $h_\ell = 0.75 \sum_{i \in I} H_{\ell i}$. For the first set of the follower's constraints we have $\tilde{f}_k = 0.25\big(\sum_{i \in I} \tilde{L}_{ki} + \sum_{j \in J} \tilde{F}_{kj}\big)$, where $k \in \{1, \ldots, \tilde{m}\}$ and $J = \{1, \ldots, n\}$. The performance of the proposed formulations are presented in Tables 6 and 7 for problems with $\mathbb{X} = \mathbb{Z}^q_+$ and in Tables 8 and 9 for problems with $\mathbb{X} = \{0,1\}^q$. In contrast to Tables 7 - 9, we do not include the last two rows in Table 6, because none of the proposed reformulations can solve these problem sizes within the time limit.

Table 5: The sizes of the proposed reformulations for **BBLIP**, where p and q represent the leader's number of constraints and variables, respectively, $\tilde{m}$ is the number of constraints given by matrices $\tilde{F}$ and $\tilde{L}$, and n is the number of the follower's variables. Parameter $\bar{R}$ is equal to $\sum \lfloor \log_2(U_i) \rfloor + q$, where U_i is a valid upper bound for the value of x_i.

Formulation		# Continuous variables	# Discrete variable	# Linear constraints
$x \in \mathbb{Z}_+^q$	**R1**	$2n + \tilde{m}$	$q + 2n + \tilde{m}$	$p + 3\tilde{m} + 6n$
	R2	$2n + \tilde{m} + \tilde{m}\bar{R}$	$q + \bar{R}$	$p + q + \tilde{m} + 2n + 4\tilde{m}\bar{R} + 1$
	R3	$2n + \tilde{m} + \bar{R}$	$q + \bar{R}$	$p + q + \tilde{m} + 2n + 4\bar{R} + 1$
$x \in \{0,1\}^q$	**R1**	$2n + \tilde{m}$	$q + 2n + \tilde{m}$	$p + 3\tilde{m} + 6n$
	R2	$2n + \tilde{m} + \tilde{m}q$	q	$p + \tilde{m} + 2n + 4\tilde{m}q + 1$
	R3	$2n + \tilde{m} + q$	q	$p + \tilde{m} + 2n + 4q + 1$

The results reported in Tables 6-9 show that **R2** and **R3** perform better than **R1** in terms of their running times for most instances (except some cases in Tables 6 and 7). In particular, when the value of $\tilde{m}$ increases to 10 or 15, **R1** is unable to find an optimal solution for most instances, while both **R2** and **R3** are capable of handling these instances.

When comparing **R2** and **R3** we observe that for both cases $x \in \mathbb{Z}_+^q$ and $x \in \{0,1\}^q$, the running time of **R3** is better than the running time of **R2**. This difference becomes more noticeable when the value of $\tilde{m}$ increases, which can be explained by comparing the sizes of the reformulations in Table 5.

The quality of LP relaxation in **R1** is typically better than the quality of LP relaxations of **R2** and **R3**. The required conditions of Proposition 22 do not hold in Tables 6-9. That is, $\Theta_i^U \leq \sum_{k\in K} L_{ki}\theta_k^U$ for some $i \in I$. However, the results in these tables suggest that there is no significant differences between **R2** and **R3** in terms of the quality of their LP relaxations.

4.3.2 BLIPs with Interdiction Constraints (BLIPI)

In this section we consider a class of **BLIP**s, where the leader's actions are restricted to "interdict," (i.e., block) a subset of the follower's variables. There are several variations of this class of problems including classical problems such as finding the k-most vital arcs of a

Table 6: Results for **BBLIP** with $\mathbb{X} = \mathbb{Z}_+^q$ and $p = 1$: the average running times (in seconds) and the LP relaxation quality given by ζ_{LP}^*/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, n, p, $\tilde{m}$	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
10-100-1-5	28	**1.300**	57.1	1.301	**16.5**	1.301
10-100-1-10	5188.4	**1.278**	89.5	1.282	**20.2**	1.282
10-100-1-15	-	**1.289**	144.8	1.292	**24**	1.292
10-150-1-5	107.3	**1.335**	124.5	1.342	**52.8**	1.342
10-150-1-10	-	**1.398**	193.9	1.405	**62.2**	1.405
10-150-1-15	-	**1.376**	388.1	1.382	**89.8**	1.381
10-200-1-5	824.4	1.368	210.5	1.369	**108.2**	**1.367**
10-200-1-10	-	**1.409**	377.2	1.417	**126.4**	1.417
10-200-1-15	-	**1.428**	425.7	1.434	**109.6**	1.434
15-100-1-5	**20.9**	**1.227**	4448	1.232	1959.1	1.233
15-100-1-10	5142	**1.267**	9347.1	1.272	**3496.4**	1.273
15-100-1-15	-	**1.237**	-	1.242	**4495.1**	1.241
15-150-1-5	**235**	**1.305**	-	1.311	5344.6	1.311
15-150-1-10	-	1.295	-	**1.202**	**6863.9**	1.301
15-150-1-15	-	**1.337**	-	1.342	**7773.3**	1.343
15-200-1-5	**1194.8**	**1.315**	-	1.335	5987.9	1.321

network (see, e.g., [39, 51]), as well as more recent examples in defending critical infrastructure [27], matching interdiction in bipartite graphs [118], and bilevel knapsack problems with interdiction constraints [32, 44]. Here, we consider two versions of **BLIPI**, where the lower-level problem is an LP, while the upper-level decision variables are either general integers or binary. Formally, the formulation of the problem is given by:

$$[\textbf{BLIPI}] \quad \min_{x \in \mathbb{X}} \quad \boldsymbol{a}^\top x + \boldsymbol{d}^\top y \tag{4.13a}$$

$$\text{subject to} \quad \boldsymbol{H} x \geq \boldsymbol{h}, \tag{4.13b}$$

$$x \leq u, \tag{4.13c}$$

$$y \in \operatorname*{argmax}_{\hat{y} \in \mathbb{R}_+^n} \{\boldsymbol{c}^\top \hat{y} : \tilde{\boldsymbol{F}} \hat{y} \leq \tilde{\boldsymbol{f}},\ \boldsymbol{I} \hat{y} \leq \tilde{\boldsymbol{U}} x\} \tag{4.13d}$$

Table 7: Results for **BBLIP** with $\mathbb{X} = \mathbb{Z}_+^q$ and $p = 10$: the average running times (in seconds) and the LP relaxation quality given by ζ_{LP}^*/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, n, p, $\tilde{m}$	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
10-100-10-5	23.8	**1.429**	1.9	1.436	1.9	1.435
10-100-10-10	-	**1.444**	3.9	1.451	**1.9**	1.450
10-100-10-15	-	1.402	6.2	**1.401**	**2.5**	1.406
10-150-10-5	217.4	**1.412**	2.9	1.420	**2.4**	1.416
10-150-10-10	-	**1.421**	4.7	1.428	**2.6**	1.425
10-150-10-15	-	**1.474**	8.5	1.482	**3.3**	1.480
10-200-10-5	1651.1	**1.496**	4.2	1.505	**3.2**	1.500
10-200-10-10	-	**1.519**	6.8	1.528	**3.6**	1.525
10-200-10-15	-	**1.489**	10	1.497	**3.6**	1.494
15-100-10-5	**41**	**1.315**	349.3	1.320	194.5	1.321
15-100-10-10	-	**1.309**	598.3	1.312	**186.2**	1.313
15-100-10-15	-	**1.301**	723.6	1.305	**225.1**	1.305
15-150-10-5	419.5	**1.416**	661.9	1.422	**248.4**	1.422
15-150-10-10	-	**1.428**	1136.9	1.435	**433.8**	1.434
15-150-10-15	-	**1.370**	1421.7	1.375	**439.8**	1.375
15-200-10-5	2875.8	**1.417**	593.2	1.426	**337.6**	1.422
15-200-10-10	-	**1.458**	1358	1.465	**470.7**	1.463
15-200-10-15	-	**1.500**	1771	1.507	**448.4**	1.506

where $\boldsymbol{H} \in \mathbb{R}^{p\times n}$ and $\tilde{\boldsymbol{F}} \in \mathbb{R}^{\tilde{m}\times n}$. If it is assumed that $\mathbb{X} = \mathbb{Z}_+^n$, then $\tilde{\boldsymbol{U}}$ is an identity matrix; if $\mathbb{X} = \{0,1\}^n$, then $\tilde{\boldsymbol{U}}$ is a diagonal matrix whose j-th entry provides an upper-bound on the value of y_j, $j \in J$. Clearly, **BLIPI** can also be framed in terms of problem (4.1) with $q = n$ and $m = \tilde{m} + n$.

In Table 10 we compare the size of the proposed reformulations for both integer and binary versions. In this problem, however, it is readily seen that $K = I \cup \{1, \ldots, \tilde{m}\}$ and $\sum_{k\in K} L_{ki}\theta_k = -\theta_i$ for all $i \in I$ in the integer case, while $\sum_{k\in K} L_{ki}\theta_k = -\widetilde{U}_{ii}\theta_i$ for the binary case. Thus, reformulations **R2** and **R3** are equivalent as the linear combination $\sum_{k\in K} L_{ki}\theta_k$ consists of a single variable.

Table 8: Results for **BBLIP** with $\mathbb{X} = \{0,1\}^q$ and $p = 1$: the average running times (in seconds) and the LP relaxation quality given by ζ^*_{LP}/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, n, p, $\tilde{m}$	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
10-100-1-5	14.6	**1.417**	0.5	1.425	**0.1**	1.425
10-100-1-10	-	**1.452**	0.8	1.461	**0.3**	1.460
10-100-1-15	-	**1.400**	1.1	1.507	**0.7**	1.501
10-150-1-5	81	**1.533**	0.8	1.544	**0.3**	1.543
10-150-1-10	-	**1.481**	0.8	1.488	**0.4**	1.488
10-150-1-15	-	**1.549**	1.5	1.557	**0.5**	1.557
10-200-1-5	794.8	**1.540**	0.8	1.551	0.8	1.550
10-200-1-10	-	**1.556**	1.1	1.566	**0.5**	1.565
10-200-1-15	-	**1.553**	1.6	1.561	**0.9**	1.561
15-100-1-5	20.2	**1.403**	5.2	1.410	**1.4**	1.411
15-100-1-10	-	**1.400**	7.2	1.406	**2.7**	1.401
15-100-1-15	-	**1.406**	8.8	1.412	**3.1**	1.412
15-150-1-5	82.8	**1.419**	6	1.427	**3.5**	1.427
15-150-1-10	-	**1.436**	9.7	1.443	**5.1**	1.443
15-150-1-15	-	**1.536**	14.3	1.543	**6.2**	1.543
15-200-1-5	1451	**1.483**	6.6	1.494	**4.4**	1.494
15-200-1-10	-	**1.506**	11.2	1.515	**7**	1.515
15-200-1-15	-	**1.476**	17.6	1.485	**8.3**	1.485

All elements of $\boldsymbol{a}$, $\boldsymbol{d}$, $\boldsymbol{H}$, $\tilde{\boldsymbol{F}}$, $\tilde{\boldsymbol{f}}$, and $\boldsymbol{c}$ in the test instances are randomly generated from a uniform $U[1, 50]$ distribution, and as such all entries are non-zero. For any leader constraint ℓ, $\ell = 1, \ldots, p$, we have $h_\ell = 3\sum_{i \in I} H_{\ell i}$ for $x \in \mathbb{Z}^n_+$ and $h_\ell = 0.4\sum_{i \in I} H_{\ell i}$ for $x \in \{0,1\}^n$. Moreover, for any follower's constraint $k = 1, \ldots, \tilde{m}$ we have $\tilde{f}_k = \sum_{j \in J} \tilde{F}_{kj}$ for $x \in \mathbb{Z}^n_+$, and $\tilde{f}_k = 2\sum_{j \in J} \tilde{F}_{kj}$ for $x \in \{0,1\}^n$. We assume an upper bound on the leader's variables of 10 in the integer case, i.e., $u_i = 10$ for all $i \in I$, while in the binary case $u_i = 1$ for all $i \in I$. Moreover, we assume that $\widetilde{U}_{ii} = 1000$ for all $i \in I$. The performance of the proposed formulations is compared in Tables 11 and 12 for the integer and binary cases, respectively.

Table 9: Results for **BBLIP** with $\mathbb{X} = \{0, 1\}^q$ and $p = 10$: the average running times (in seconds) and the LP relaxation quality given by ζ^*_{LP}/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, n, p, $\tilde{m}$	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
10-100-10-5	16.9	**1.440**	0.5	1.448	**0.6**	1.447
10-100-10-10	-	**1.420**	1	1.427	**0.3**	1.427
10-100-10-15	-	**1.437**	0.8	1.443	**0.6**	1.442
10-150-10-5	62.5	**1.454**	0.6	1.463	**0.4**	1.462
10-150-10-10	-	**1.529**	1.1	1.537	**0.7**	1.536
10-150-10-15	-	**1.532**	1.6	1.540	**0.9**	1.540
10-200-10-5	1084.7	**1.506**	1.3	1.516	**0.5**	1.515
10-200-10-10	-	**1.530**	1.2	1.539	**0.4**	1.537
10-200-10-15	-	**1.516**	2.1	1.523	**0.9**	1.523
15-100-10-5	21.8	**1.440**	4.7	1.447	**1.3**	1.447
15-100-10-10	-	**1.473**	7.5	1.479	**2.5**	1.479
15-100-10-15	-	**1.445**	10.9	1.451	**3.8**	1.451
15-150-10-5	126.1	**1.484**	6.8	1.494	**3.3**	1.494
15-150-10-10	-	**1.490**	9.9	1.497	**5.3**	1.497
15-150-10-15	-	**1.478**	14.1	1.486	**6.5**	1.485
15-200-10-5	1551.4	**1.512**	7.1	1.522	**4.2**	1.521
15-200-10-10	-	**1.425**	12	1.534	**6.4**	1.533
15-200-10-15	-	**1.500**	17.5	1.508	**8.1**	1.508

From the results reported in Table 11, it can be seen that the running time of **R1** for $\tilde{m} = 70$ is significantly larger than its running time for $\tilde{m} = 15$ and $\tilde{m} = 30$. This observation follows from the fact that the number of constraints and discrete variables in **R1** grows as the value of $\tilde{m}$ increases, see Table 10. In contrast, the number of discrete variables in **R2** is independent from $\tilde{m}$. Also, we note that in Table 11 the qualities of LP relaxations of **R1** and **R2** are rather close. Therefore, **R2** outperforms **R1** with respect to the running time as $\tilde{m}$ increases to 70 in Table 11.

Similar observations hold for Table 12 for smaller values of n. However, for $n = 80$ the quality of the LP relaxation of **R2** is much worse than that of **R1**. Consequently, the per-

Table 10: The sizes of the proposed reformulations for **BLIPI**, where p and n represent the leader's number of constraints and variables, respectively, $\tilde{m}$ is the number of constraints given by matrices $\tilde{F}$ and $\tilde{L}$, and n is the number of the follower's variables. Parameter $\bar{R}$ is equal to $\sum \lfloor \log_2(U_i) \rfloor + q$, where U_i is a valid upper bound for the value of x_i.

	Formulation	# Continuous variables	# Discrete variable	# Linear constraints
$x \in \mathbb{Z}^n_+$	**R1**	$2n + \tilde{m}$	$3n + \tilde{m}$	$p + 3\tilde{m} + 7n$
	R2	$2n + \tilde{m} + \bar{R}$	$n + \bar{R}$	$p + \tilde{m} + 4n + 4\bar{R} + 1$
$x \in \{0,1\}^n$	**R1**	$2n + \tilde{m}$	$3n + \tilde{m}$	$p + 3\tilde{m} + 7n$
	R2	$3n + \tilde{m}$	n	$p + \tilde{m} + 7n + 1$

formance of **R2** significantly deteriorates in terms of the running time, and **R1** outperforms **R2** for $n = 80$ in Table 12. Moreover, **R2** cannot solve the last two problem sizes in Table 12 within the time limit, while **R1** can handle those.

4.3.3 Bilevel Facility Location Problem (BFLP)

We consider a version of the facility location problem in a decentralized manufacturing setting, see [30]. A firm that produces a set of products given by $\mathcal{G}$ can place new facilities in the locations given by $I = \{1, \ldots, q\}$. The leader chooses the facilities placement, while the follower must determine the fraction of each product's demand that each facility processes. The firm incurs a cost of $a_i^{(1)}$ for each facility opened at location $i \in I$, and incurs an opportunity cost of $a_i^{(2)}$ for each unused production capacity of any plant in location $i \in I$ after it is opened. The follower faces a cost of $c_i^{(1)}$ for using a unit of capacity at a facility in location $i \in I$, and a cost of $c_{ig}^{(2)}$ associated with the transportation of $g \in \mathcal{G}$ from a facility in location $i \in I$.

Let x_i be the number of facilities to open at location i, and let y_{ig} be the fraction of the demand for product g that the plants in location i process. If d_g denotes the demand for g, r_{ig} is the units of capacity needed to make product g at a facility in location i, and C_i is

Table 11: Results for **BLIPI** with $\mathbb{X} = \mathbb{Z}^n_+$: the average running times (in seconds) and the LP relaxation quality given by ζ^*_{LP}/ζ^*. The value in **bold** represents the best result for each row across both reformulations.

	R1		**R2**	
n, p, $\tilde{m}$	Time	LP Qual	Time	LP Qual
25-5-15	**2.1**	0.723	8.5	0.723
25-5-30	**3.4**	0.668	9.8	0.6668
25-5-70	34	0.751	**10.5**	0.751
25-15-15	**3.1**	0.699	14.2	0.699
25-15-30	**5.9**	0.736	19.8	0.736
25-15-70	200.1	0.667	**15.2**	0.667
40-5-15	**3.9**	**0.681**	326.4	0.679
40-5-30	**10.7**	**0.688**	652.5	0.684
40-5-70	765.6	**0.668**	**290.9**	0.661
40-15-15	**17.2**	**0.741**	1356.6	0.687
40-15-30	**160**	**0.752**	1903.2	0.714
40-15-70	2176.6	**0.748**	**829.4**	0.646
55-5-15	**11.7**	**0.757**	2481.8	0.683
55-5-30	**182.9**	**0.705**	2369.9	0.669
55-5-70	3685	**0.700**	**2177.4**	0.656
55-15-15	**49.6**	**0.713**	4136.8	0.682
55-15-30	**1041.4**	0.698	4405.8	0.698
55-15-70	9475	0.680	**6227.5**	0.680

the capacity of a plant at location i, then the firm facility location problem is given by the following bilevel problem:

$$[\textbf{BFLP}]\ \min_{x\in\mathbb{X}} \sum_{i\in I} a_i^{(1)} x_i + \sum_{i\in I} a_i^{(2)} \Big(C_i x_i - \sum_{g\in\mathcal{G}} d_g r_{ig} y_{ig} \Big) \tag{4.14a}$$

$$\text{subject to} x_i \leq Q \quad \forall i \in I \tag{4.14b}$$

$$y \in \text{argmin} \sum_{i\in I} \sum_{g\in\mathcal{G}} (c_i^{(1)} r_{ig} + c_{ig}^{(2)}) d_g \hat{y}_{ig} \tag{4.14c}$$

$$\text{s.t.} \ \sum_{i\in I} \hat{y}_{ig} = 1 \qquad \forall g \in \mathcal{G} \tag{4.14d}$$

$$\sum_{g\in\mathcal{G}} d_g r_{ig} \hat{y}_{ig} \leq C_i x_i \qquad \forall i \in I \tag{4.14e}$$

Table 12: Results for **BLIPI** with $\mathbb{X} = \{0,1\}^n$: the average running times (in seconds) and the LP relaxation quality given by ζ^*_{LP}/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**	
n, p, $\tilde{m}$	Time	LP Qual.	Time	LP Qual.
55-5-15	**7.3**	**0.271**	14.6	0.191
55-5-30	178.1	**0.301**	**28.9**	0.218
55-5-70	401.8	**0.336**	**26.9**	0.225
55-15-15	**24**	**0.261**	56.8	0.195
55-15-30	296.1	**0.307**	**78.2**	0.224
55-15-70	1207.4	**0.319**	**56.5**	0.216
65-5-15	**6.7**	**0.326**	222.3	0.192
65-5-30	**132.7**	**0.365**	521	0.200
65-5-70	1541	**0.422**	**325.7**	0.222
65-15-15	**24.6**	**0.327**	481.4	0.206
65-15-30	**340.8**	**0.346**	504.5	0.202
65-15-70	3753.6	**0.388**	**1314.9**	0.228
80-5-15	**7.1**	**0.435**	642.6	0.183
80-5-30	**186.1**	**0.451**	2595.6	0.205
80-5-70	**2344.9**	**0.503**	3680.2	0.204
80-15-15	**42.4**	**0.442**	4974.2	0.214
80-15-30	**1239.4**	**0.453**	-	0.195
80-15-70	**6625.9**	**0.488**	-	0.210

$$\sum_{g \in \mathcal{G}} \hat{y}_{ig} \leq G x_i \qquad \forall i \in I \tag{4.14f}$$

$$\hat{y}_{ig} \geq 0 \qquad \forall i \in I,\ \forall g \in \mathcal{G}, \tag{4.14g}$$

where in equation (4.14b) $\mathbb{X}$ can be either $\mathbb{Z}^q_+$ or $\{0,1\}^q$, Q is the maximum number of facilities that can be opened at any given location ($Q = 1$ if $\mathbb{X} = \{0,1\}^q$) and $G = |\mathcal{G}|$.

Let $\bar{Q} = \lfloor \log(Q) \rfloor + 1$. Observe that in this problem $p = 0$ if $\mathbb{X} = \{0,1\}^q$ and $p = q$, otherwise. Furthermore, $m = G + 2q$, $n = qG$ and $\bar{R} = q\bar{Q}$. The sizes of the reformulations are summarized in Table 13.

We generate instances with the number of locations q given by 20, 30, and 40, while the number of products G take values $G = qs$, with $s = 1, \ldots, 6$. For the integer case we assume

Table 13: The sizes of the proposed reformulations for **BFLP**, where q represent the number of potential locations (the number of leader's variables) and G is the number of products, respectively. Parameter $\bar{Q}$ is equal to $\lfloor \log(Q) \rfloor + 1$ where Q is the maximum number of facilities that can be opened at any given location.

Formulation		# Continuous variables	# Discrete variable	# Linear constraints
$x \in \mathbb{Z}_+^q$	**R1**	$q(G+2)+G$	$q(G+3)+G$	$q(3G+7)+3G$
	R2	$q(G+2+G\bar{Q}+2q\bar{Q})+G$	$q(1+\bar{Q})$	$q(G+4+4G\bar{Q}+8q\bar{Q})+G+1$
	R3	$q(G+\bar{Q}+2)+G$	$q(1+\bar{Q})$	$q(G+4+4\bar{Q})+G+1$
$x \in \{0,1\}^q$	**R1**	$q(G+2)+G$	$q(G+3)+G$	$q(3G+6)+3G$
	R2	$2q(G+q+1)+G$	q	$q(5G+8q+2)+G+1$
	R3	$q(G+3)+G$	q	$q(G+6)+G+1$

that the maximum number of facilities that can be opened at any location is $Q = 5$. The remaining parameter values are drawn from discrete uniform distribution $U[1, D]$, where the upper bounds D are summarized in Table 14.

Table 14: Upper bounds D of the uniform random variables that are used to generate the parameters of **BFLP**.

Model/Parameter	$a_i^{(1)}$	$a_i^{(2)}$	C_i	d_g	$c_i^{(1)}$	$c_{ig}^{(2)}$
$x \in \mathbb{Z}_+^q$	500	5	10	40	5	5
$x \in \{0,1\}^q$	50	5	10	20	10	5

Given the test instances described above, Tables 15 and 16 provide the results of our experiments. For both general integer and binary cases, reformulation **R3** is the best one with respect to average running times, being orders of magnitude better than **R1**, and also

Table 15: Results for **BFLP** with $\mathbb{X} = \mathbb{Z}_+^q$: the average running times and the LP relaxation quality given by ζ_{LP}^*/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, G	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
20-20	0.6	0.688	2.4	0.688	**0.4**	0.688
20-40	3.9	0.538	3.8	0.538	**0.8**	0.538
20-60	7.2	0.496	4.2	0.496	**0.6**	0.496
20-80	13.5	0.568	8.4	0.568	**0.8**	0.568
20-100	25.9	0.609	11.2	0.609	**1**	0.609
20-120	43.2	0.668	8.2	0.668	**0.9**	0.668
30-30	2.1	0.671	4.6	0.671	**0.1**	0.671
30-60	25.7	0.521	16.9	0.521	**0.8**	0.521
30-90	27.9	0.554	16.7	0.554	**1**	0.554
30-120	78.6	0.634	27.6	0.634	**2**	0.634
30-150	255.5	0.606	37.1	0.606	**3.3**	0.606
30-180	1106.2	0.697	48.7	0.697	**3**	0.697
40-40	5.9	0.594	11.6	0.594	**0.8**	0.594
40-80	29.9	0.596	43.6	0.596	**1.8**	0.596
40-120	112.9	0.590	43.7	0.590	**2.6**	0.590
40-160	465	0.584	113.8	**0.617**	**6**	**0.617**
40-200	-	-	242.3	0.555	**11.6**	0.555
40-240	-	-	392	0.634	**22.5**	0.634

far better than **R2**. In particular, the superiority of **R3** and **R2** with respect to **R1** can be explained by the fact that **R3** and **R2** have far less discrete variables than **R1**, see Table 13. In addition, we observe that the LP relaxation qualities associated with each of the reformulations are fairly similar (**R2** and **R3** being slightly better than **R1**).

Finally, we observe that the constraints in (4.14f) can be replaced by the constraints $y_{ig} \leq x_i$ for all $i \in I$ and $g \in \mathcal{G}$; such a 'disaggregated' formulation gives a stronger LP relaxation to all the reformulations. In our experiments, however, we use the aggregated version as this is the formulation that is originally presented in [30].

Note that in the disaggregated problem, reformulation **R1** adds new binary variables to account for the linearization of the new complementary slackness constraints. As a consequence, in this reformulation there is a tradeoff between the strength of formulation and the number of auxiliary binary variables that need to be introduced. In contrast, the disaggregated versions of **R2** and **R3** do not add any new constraints or variables (besides the disaggregated constraints).

Table 16: Results for **BFLP** with $\mathbb{X} = \{0,1\}^q$: the average running times (in seconds) and the LP relaxation quality given by ζ^*_{LP}/ζ^*. The value in **bold** represents the best result for each row across all reformulations and symbol '-' indicates that an optimal solution was not found within the time limit for at least one of the instances.

	R1		**R2**		**R3**	
q, G	Time	LP Qual.	Time	LP Qual.	Time	LP Qual.
20-20	0.9	0.331	0.8	**0.458**	**0.2**	**0.458**
20-40	4.6	0.253	1.9	**0.316**	**0.2**	**0.316**
20-60	74.1	0.352	2.5	**0.446**	**0.4**	**0.446**
20-80	41.3	0.312	3.4	**0.456**	**0.9**	**0.456**
20-100	56.2	0.253	3.9	**0.271**	**1**	**0.271**
20-120	74.6	0.417	5.3	**0.421**	**1.1**	**0.421**
30-30	6.5	0.306	3.2	**0.340**	**0.4**	**0.340**
30-60	35.2	0.438	5.1	**0.483**	**0.6**	**0.483**
30-90	771.8	0.424	11.6	**0.510**	**1.1**	**0.510**
30-120	-	-	13.4	**0.427**	**2.5**	**0.427**
30-150	269.7	0.397	15.6	**0.461**	**2.3**	**0.461**
30-180	2447.9	0.355	15.9	**0.503**	**3.1**	**0.503**
40-40	23.1	0.378	5.3	**0.386**	**0.8**	**0.386**
40-80	157.4	0.359	9.5	**0.417**	**1.6**	**0.417**
40-120	638.6	0.300	14.1	**0.347**	**3.2**	**0.347**
40-160	1334.4	0.281	47.3	**0.392**	**5.5**	**0.392**
40-200	-	-	57.8	**0.399**	**8.3**	**0.399**
40-240	-	-	100.5	**0.477**	**20.3**	**0.477**

4.4 CONCLUSION

In this note we considered single-level reformulations of a class of bilevel linear integer programs. Along with applying KKT optimality conditions, strong duality can be employed for deriving such reformulations under the assumption that the upper-level variables are discrete. In some settings these SD-based reformulation may reduce the number of variables and constraints significantly with respect to the KKT-based reformulation, and more importantly, make the number of binary variables independent of the size of the lower-level problem. We performed numerical experiments with three classes of bilevel problems to explore the performances of an off-the-shelf MIP solver with these reformulations. Our experiments show that the SD-based reformulations (in particular, **R3**) can lead to orders of magnitude reduction in computational times for certain classes of problems.

We note that there are several factors that play a role in the speed at which an MIP is solved, with two of the most important ones being the size of the problem (the number of variables and constraints), and the tightness of the linear programming relaxations. In the instances where the SD-based reformulations outperform the KKT-based reformulations, the reformulations have somewhat comparable LP relaxation qualities, but the SD-based reformulations have clearly fewer discrete variables. We believe that this difference is the key factor that may reduce the computational times of the SD-based reformulations.

Although our experiments are limited to particular instances, given the above observations, we believe that the considered SD-based formulations can be useful in problems where the KKT-based reformulation introduces significantly more discrete variables than the SD-based ones. In particular, this holds true for bilevel problems where the number of constraints and variables of the lower-level problem is much larger than the number of variables of the upper-level problem.

5.0 ON BILEVEL MODELS FOR PEDIATRIC VACCINE PRICING PROBLEM

5.1 INTRODUCTION

Routine vaccination is a crucial factor for preventing pediatric infectious diseases from spreading. With the goal of protecting public health and safety in the United States, the Centers for Disease Control and Prevention (CDC) prescribes relevant immunization guidelines to ensure timely and accurate vaccine administration, see, e.g., [37]. In particular, the Advisory Committee of Immunization practices (ACIP) of the CDC, along with American Academy of Pediatrics (AAP) and American Academy of Family Physicians (AAFP), annually publishes the recommended childhood immunization schedule (RCIS) [37]. This schedule is designed to protect infants and children from serious diseases and specifies the age range when each vaccine is recommended [35].

The robustness and reliability of the pediatric vaccine market is an essential element to keep immunization coverage at appropriate levels. Vaccine manufacturers play a principal role in this market by providing the required supply in a timely manner. However, because of the challenging nature of the pediatric vaccine industry, only a few pharmaceutical companies actively participate in vaccine production and distribution in the United States market. Moreover, limited demands and rising participation costs make this industry less attractive and as a result many companies have left the pediatric vaccine market in the United States [96]. Therefore, because of the importance of immunization coverage to national public health, many experts argue that vaccine manufacturers must receive financial incentives to remain in the market [62, 80, 85, 90].

In particular, in [80] the author proposes an economic model for the vaccine pricing problem and incorporates different financial incentives for manufacturers into the model. Similarly, [5] considers different incentives for manufacturers and consumers in order to motivate them to cooperate in the vaccine market. A pricing model is proposed in [62] which sets the prices of vaccines based on their societal values before their production. Furthermore, [74] develops a model that maximizes the net profit of all pharmaceutical companies involved and minimizes their total costs. A mixed integer nonlinear program for the vaccine pricing problem is developed in [94] that assures a minimum profit level for all manufacturers. Moreover, a game theory approach is developed in [20] and [95] to explore different pricing strategies in the vaccine market.

To ensure proper vaccine coverage for a single child and public health protection, health care providers purchase and administer pediatric vaccines based on the RCIS. This is a complex encounter because new diseases are added to the RCIS each year and also, new multivalent vaccines are designed by manufacturers to protect children against more pediatric diseases. Indeed, during the past 25 years, RCIS has significantly changed and it requires now that children receive multiple injections. In this regard, [69] and [110] develop an integer program to find a set of vaccines that minimize the cost to fully immunize a child according to a given RCIS. This set is called *the minimum cost formulary.* In addition, [100] and [99] develop a mechanism to compute a vaccine's *maximum inclusion price.* This is the maximum price at which a vaccine is included in the minimum cost formulary. A similar study is presented in [70].

The most relevant study to our work in this chapter is presented in [96], where the authors model the pediatric vaccine pricing problem as a bilevel nonlinear program. They model the pricing problem from the perspective of a single manufacturer who sets the prices to maximize its profit in an oligopolistic market, assuming that the prices of vaccines produced by the competitors are given. In this chapter we study the pediatric vaccine pricing problem in a setting similar to [96]. Specifically, we formulate the problem as a mixed-integer nonlinear bilevel program, where at the upper level, the manufacturer sets the the prices of vaccines and at the lower level, a potential purchaser, e.g., health care providers, seeks to minimize the cost of satisfying a given RCIS. That is, the purchaser have to decide whether to buy vaccines from the manufacturer or other producers in the market, i.e., competitors. The presence of binary variables in the lower-level problem along with the nonlinear term in the upper- and lower-level objective functions, make this bilevel program difficult to solve.

Our main contribution in this chapter is to model and solve the pediatric vaccine pricing problem in a setting where the prices of vaccines produced by the competitors are nondeterministic. In the related literature, see, e.g., [96], it is assumed that the prices of vaccines produced by the competitors are known exactly in advance. However, in reality these values may involve uncertainties. We propose two robust formulations for the pediatric vaccine pricing problem, where the market prices of vaccines manufactured by competitors are given by some uncertainty sets. Furthermore, we present an exact solution approach for this class of problems and illustrate the results. Our approach finds an optimal solution of the problem developed in [96]. Note that, the latter study describes only heuristic solution approaches. Our numerical results shows that, compared to the existing approaches in the literature, our robust models may improve the manufacturer's profit in nondeterministic settings, where the vaccine prices of competitor manufacturers are not precisely known.

The remainder of this chapter is organized as follows. In Section 5.2 we describe robust bilevel formulations for the pediatric vaccine pricing problem. In Section 5.3 we develop an exact solution method to solve the proposed robust models. Then in Section 5.4 we provide our numerical experiments and discuss the results obtained. Finally, Section 5.5 includes our final remarks and conclusion.

5.2 PROBLEM STATEMENT

Different forms of the Pediatric Vaccine Pricing Problem (**PVPP**) are studied in the literature [20, 62, 95]. We consider this problem from a single manufacturer's point of view and formulate it as a mixed-integer nonlinear bilevel program. This bilevel formulation is originally developed in [96] where the authors propose different heuristic algorithms as solution methods. The leader in this bilevel problem is a manufacturer who controls the prices of a set of vaccines to maximize her/his profit. When the prices are set, the purchaser, i.e., the follower, decides who to buy vaccines from, with the goal of minimizing the vaccination cost to satisfy a given RCIS. First, we introduce the necessary notation to present the model (we follow the notation from [96]).

Parameters:

$T = \{1, 2, \ldots, \tau\}$: set of time periods for a given RCIS.

$D = \{1, 2, \ldots, \delta\}$: set of diseases which require immunization.

$V = \{1, 2, \ldots, \upsilon\}$: set of vaccines produced by the manufacturer.

$\bar{V} = \{1, 2, \ldots, \bar{\upsilon}\}$: set of vaccines produced by the competitors.

n_d: number of vaccine doses needed for immunization against disease $d \in D$ in RCIS.

c_v: cost of producing vaccine $v \in V$.

k: injection cost incurred by health care provider.

f_v: vaccine-specific cost incurred by provider to administer vaccine $v \in V$.

$\bar{f}_v$: vaccine-specific cost incurred by provider for vaccine $v \in \bar{V}$.

q_v: price of vaccine $v \in \bar{V}$ sold by other manufacturers.

I_{vd}: binary parameter indicating if vaccine $v \in V$ immunizes against disease $d \in D$.

$\bar{I}_{vd}$: binary parameter indicating if vaccine $v \in \bar{V}$ immunizes against disease $d \in D$.

J_{tv}: binary parameter indicating if vaccine $v \in V$ can be administered at time $t \in T$.

$\bar{J}_{tv}$: binary parameter indicating if vaccine $v \in \bar{V}$ can be administered at time $t \in T$.

S_{djt}: binary parameter indicating if in time t, a vaccine may be administered to satisfy the j-th dose required for disease $d \in D$, $j = 1, 2, \ldots, n_d$.

Q_{tv}: binary parameter indicating if a purchaser must pay for vaccine $v \in V$ to be administered in time period $t \in T$. Note that $Q_{tv} = 1$ for most vaccines v, except for a special situation where purchaser does not need to pay for a vaccine.

$\bar{Q}_{tv}$: binary parameter indicating if a purchaser must pay for vaccine $v \in \bar{V}$ to be administered in time period $t \in T$.

Decision variables. Let p_v be the price of vaccine $v \in V$, determined by the manufacturer (the leader). Once the prices are set, the customer (the follower), e.g., health care provider, purchases and administers vaccines based on the specified schedule in RCIS. Let

x_{tv} be the customer's binary decision variable which is 1 iff vaccine $v \in V$ is administered at time period $t \in T$. Similarly, y_{tv} is 1 iff vaccine $v \in \bar{V}$ is administered in time period $t \in T$.

Thus, **PVPP** can be modeled as the following bilevel nonlinear mixed-integer program:

$$[\mathbf{PVPP}]: \max_{\mathbf{p} \in \mathbb{R}_+^{|V|}} f(\mathbf{p}, \mathbf{x}) = \sum_t \sum_{v \in V} (p_v - c_v) Q_{tv} x_{tv} \tag{5.1a}$$

$$\text{subject to } \mathbf{x}, \mathbf{y} \in \operatorname*{argmin}_{\hat{\mathbf{x}}, \hat{\mathbf{y}}} \sum_t \Big(\sum_{v \in V} (p_v + f_v + k) Q_{tv} \hat{x}_{tv} + \sum_{v \in \bar{V}} (q_v + \bar{f}_v + k) \bar{Q}_{tv} \hat{y}_{tv} \Big), \tag{5.1b}$$

$$\text{subject to } 1 - \sum_t S_{djt} \Big(\sum_{v \in V} I_{vd} J_{tv} \hat{x}_{tv} + \sum_{v \in \bar{V}} \bar{I}_{vd} \bar{J}_{tv} \hat{y}_{tv} \Big) \leq 0, \ \forall\, d \in D,\ j = 1, \ldots, n_d, \tag{5.1c}$$

$$g_i(\mathbf{x}, \mathbf{y}) \leq 0 \qquad \forall\, i \in N, \tag{5.1d}$$

$$x_{tv}, y_{tv} \in \{0, 1\} \quad \forall\, t \in T,\ v \in V \cup \bar{V} \tag{5.1e}$$

The manufacturer's goal is to maximize the profit per child completing a given RCIS. This profit is represented by (5.1a), where $p_v - c_v$ is the marginal profit obtained from vaccine $v \in V$. Note that, due to the presence of competitors in the vaccine market, the manufacturer's objective function is bounded. That is, for any vaccine $v \in V$, there exists a competing formulary in the market which prevents $p_v - c_v$ from being unbounded. The healthcare provider minimizes the total cost of purchasing a formulary which satisfies the RCIS. The follower's total cost, (5.1b), includes the costs of purchasing vaccines produced by the manufacturer and the competing manufacturers. The health care provider's main constraint is to satisfy the required specifications given by the RCIS. This constraint is represented in (5.1c) and it assures that the required dosages of all vaccines are administered on time. In addition, (5.1d) represents a set of side constraints specific to a vaccine formulary. For instance, this constraint prevents the health care provider from administration of two specific vaccines in the same time period.

Bilevel programs are in general quite challenging to solve. Indeed, in their simplest form, where both the upper- and lower-level problems are linear, bilevel problems are *NP*-hard [46, 61]. Thus, due to the presence of bilinear terms at both levels of **PVPP** and also because of binary variables x_{tv} and y_{tv}, it is a difficult problem to solve. In [96] it is shown that **PVPP** is an *NP*-hard problem.

A primary assumption in [96] is that the manufacturer (the leader) is aware of the vaccine prices set by the other manufacturers. That is, the value of q_v is known in advance for all vaccines $v \in \bar{V}$. In this case, the bilevel formulation (5.1) reduces to the problem discussed in [96]. We refer to this form of **PVPP** as Deterministic Pediatric Vaccine Pricing Problem (**DPVPP**) and accordingly denote its upper-level objective function by $f_d(\mathbf{p}, \mathbf{x})$.

The aforementioned assumption may be violated, in reality, as the competitors in oligopolistic markets change their prices. In this chapter we study **PVPP** in a setting where q_v, for all vaccines $v \in \bar{V}$, is a nondeterministic parameter and given by some uncertainty sets. That is, we assume that q_v is not known for the manufacturer and it can take any value within an uncertainty set. In order to incorporate this uncertainty into our model, we exploit an idea similar to the classical robust optimization approach presented in [21, 22] and develop two robust models.

Let $\bar{p}_v$ be a lower bound on the price of vaccine $v \in \bar{V}$, i.e., $q_v \geq \bar{p}_v$, referred to as the nominal price of vaccine $v \in \bar{V}$. Moreover, let δ_v be an upper bound on the price deviation of vaccine $v \in \bar{V}$ from its nominal value, i.e., $q_v - \bar{p}_v \leq \delta_v$. In our first robust approach, we assume that the total price deviation from the nominal values over all vaccines $v \in \bar{V}$, is bounded by a given value Δ, i.e., $\sum_{v \in \bar{V}} (q_v - \bar{p}_v) \leq \Delta$. Thus, we define the first uncertainty set as follows:

$$\Omega_1 = \{q_v \mid 0 \leq q_v - \bar{p}_v \leq \delta_v,\ \sum_{v \in \bar{V}} (q_v - \bar{p}_v) \leq \Delta,\ v \in \bar{V}\},$$

where $\bar{p}_v$ and δ_v are known in advance for all vaccines $v \in \bar{V}$. Obviously, if $\delta_v = 0$ for vaccine $v \in \bar{V}$, then q_v is equal to $\bar{p}_v$ and there is no uncertainty involved for vaccine v.

By definition of Ω_1, we can reformulate **PVPP** as the following robust bilevel program:

$$[\mathbf{R}^{\mathrm{I}}\text{-}\mathbf{PVPP}] : \max_{\mathbf{p}} \min_{\mathbf{q} \in \Omega_1} f_1(\mathbf{p}, \mathbf{x}) = \sum_t \sum_{v \in V} (p_v - c_v) Q_{tv} x_{tv}$$

$$\text{subject to} \quad \mathbf{x}, \mathbf{y} \in \mathcal{R}(\mathbf{p}, \mathbf{q}),$$

where $\mathbf{p} = (p_1, \dots, p_{|V|})^\top$, $\mathbf{q} = (q_1, \dots, q_{|\bar{V}|})^\top$ and $\mathcal{R}(\mathbf{p}, \mathbf{q})$ represents the follower's rational reaction set for fixed values of $\mathbf{q}$ and $\mathbf{p}$. Therefore, for given $\mathbf{p}$ and $\mathbf{q}$, set $\mathcal{R}(\mathbf{p}, \mathbf{q})$ includes the lower-level decisions $\mathbf{x}$ and $\mathbf{y}$, which satisfy constraints (5.1b)-(5.1e).

Note that this robust model generalizes formulation **PVPP** in a sense that, for $\Delta = 0$, it reduces to **PVPP**. Furthermore, by increasing the value of Δ, set Ω_1 includes more values for q_v which enables the manufacturer to take into account more uncertain scenarios with respect to the market prices. That is, a conservative manufacturer may hedge against more potential scenarios by considering a large value of Δ.

In the second robust approach, we assume that the prices of only a limited number of vaccines are deviated from their nominal values. Accordingly, we propose the second uncertainty set as follows:

$$\Omega_2 = \{q_v \mid 0 \leq q_v - \bar{p}_v \leq \delta_v z_v,\ \sum_{v \in \bar{V}} z_v \leq \Gamma,\ v \in \bar{V}\},$$

where Γ is a fixed parameter and z_v is a binary variable.

Then we reformulate our second robust bilevel model of **PVPP** as follows:

$$[\mathbf{R}^{\text{II}}\text{-}\mathbf{PVPP}] : \max_{\mathbf{p}} \min_{\mathbf{q} \in \Omega_2} f_2(\mathbf{p}, \mathbf{x}) = \sum_{t} \sum_{v \in V} (p_v - c_v) Q_{tv} x_{tv}$$
$$\text{subject to } \ \mathbf{x}, \mathbf{y} \in \mathcal{R}(\mathbf{p}, \mathbf{q})$$

This robust formulation is another generalization of **PVPP** as it reduces to **PVPP** for $\Gamma = 0$. Note that $0 \leq \Gamma \leq |\bar{V}|$ and by increasing the value of Γ, set Ω_2 can include more uncertain cases. That is, a conservative manufacturer may consider a larger value of Γ to ensure hedging against more possible scenarios. Therefore, both proposed robust formulations are generalized forms of the pediatric vaccine pricing problem developed in [96]. These models enable the manufacturer to take into account the uncertainty involved in the vaccine prices and make a more reliable pricing decision. Our uncertainty sets are motivated by approaches from the robust optimization literature, see [21, 22]. Naturally, other uncertainty sets are possible and we leave as a possible topic for future research.

Finally, we note that, for a fixed value of $\mathbf{q} \in \Omega_1 \cap \Omega_2$, $\mathbf{R}^{\text{I}}$**-PVPP**, $\mathbf{R}^{\text{II}}$**-PVPP** and **DPVPP** result in the same pricing decisions.

Proposition 23. *Let f_d^* be the optimal objective function value of* ***PVPP*** *for fixed value of* $\mathbf{q} \in \Omega_1$*,* f_1^* *and* f_2^* *be the optimal objective function value of* $\boldsymbol{R}^{\mathrm{I}}$***-PVPP*** *and* $\boldsymbol{R}^{\mathrm{II}}$***-PVPP****, respectively. Then we have that:*

$$f_1^* \leq f_d^* \quad \textit{and} \quad f_2^* \leq f_d^*$$

.

The proof is straightforward and omitted for brevity. In the next section, we propose an exact solution approach to obtain optimal solutions of these robust programs.

5.3 SOLUTION METHOD

Problem **DPVPP** is solved in [96] by applying different heuristic solution approaches that do not necessarily result in an optimal solution. In this section, first we propose an exact solution method to find the optimal solution of **DPVPP** and then, we extend this approach to solve robust models $\mathbf{R}^{\mathrm{I}}$**-PVPP** and $\mathbf{R}^{\mathrm{II}}$**-PVPP**. In the reminder of the chapter we assume the optimistic cases of the considered bilevel models.

5.3.1 Deterministic PVPP

Arguably, the most common methods of solving bilevel problems are based on reformulating them as single-level problems by replacing the linear problem (LP) at the lower level by its optimality conditions, recall our discussion in Chapter 4. However, this transformation is not applicable to (5.1) as binary variables $\mathbf{x}$ and $\mathbf{y}$ appear at the lower-level problem. Therefore, we exploit an idea similar to the exact iterative Algorithm 1 introduced in Section 3.4.1. Based on this algorithm, in each iteration we solve single-level relaxations of bilevel problem (5.1), check the optimality condition and then add a valid cut if the obtained solution is not optimal.

The single-level relaxation of (5.1) results from removing the follower's objective function, (5.1b), from **PVPP** and is given by the following problem:

$$[\mathbf{SPVPP}] : \max_{\mathbf{p},\mathbf{x},\mathbf{y}} \sum_{t}\sum_{v\in V}(p_v - c_v)Q_{tv}x_{tv}$$
$$\text{subject to } (5.1c) - (5.1e)$$

We observe that **SPVPP** is a mixed-integer bilinear problem as nonlinear term $p_v x_{tv}$ appears in the leader's objective function. However, it can be linearized by introducing new variable u_{tv} and additional set of linear constraints (see further details and discussion in [2]):

$$\big\{(x_{tv}, p_v, u_{tv}):\ u_{tv} = p_v x_{tv},\ x_{tv} \in \{0,1\},\ p_v^L \le p_v \le p_v^U\big\} =$$
$$\big\{(x_{tv}, p_v, u_{tv}):\ x_{tv} \in \{0,1\},\ p_v^L x_{tv} \le u_{tv} \le p_v^U x_{tv},\ p_v + p_v^U x_{tv} - p_v^U \le u_{tv} \le p_v + p_v^L x_{tv} - p_v^L\big\},$$

where we assume that the lower (p_v^L) and upper (p_v^U) bounds on p_v for each $v \in V$ are either readily available or can be easily computed. Hence, **SPVPP** can be re-written as an equivalent linear MIP that can be solved by a standard solver.

We employ exact Algorithm 3 to solve **DPVPP**. At each iteration, the algorithm solves **SPVPP** and checks whether or not the solution is bilevel feasible. It stops when a bilevel feasible solution is achieved. Otherwise, if the obtained solution of **SPVPP** is not bilevel feasible, the algorithm adds a valid cut to the problem and continues. The pseudo-code of the exact approach for solving **DPVPP** is provided in Algorithm 3 whose convergence is established in the next result.

Proposition 24. *Algorithm 3 finds an optimal solution for **DPVPP** in a finite number of iterations.*

We skip the proof as it is similar to the proof of Proposition 20, see Section 3.4.1. To compare the performance of Algorithm 3 against the heuristic methods developed in [96], we apply it to solve the test instances of [96] and present the results in Section 5.4.

Algorithm 3 Exact Algorithm for solving **DPVPP**

Step 1. Solve **SPVPP** and denote by $(\hat{\mathbf{p}}, \hat{\mathbf{y}}, \hat{\mathbf{x}})$ its optimal solution.

Step 2. Solve linear binary problem (5.1b)-(5.1e) for $\mathbf{p} = \hat{\mathbf{p}}$. Let $(\check{\mathbf{x}}, \check{\mathbf{y}})$ and z_f^* denote its optimal solution and the optimal objective function value, respectively.

if $z_f^* = \sum_t \Big(\sum_{v \in V} (\hat{p}_v + f_v + k) Q_{tv} \hat{x}_{tv} + \sum_{v \in \bar{V}} (q_v + \bar{f}_v + k) \bar{Q}_{tv} \hat{y}_{tv} \Big)$ **then**

$(\hat{\mathbf{p}}, \hat{\mathbf{y}}, \hat{\mathbf{x}})$ is an optimal solution of ; **STOP**.

end if

if $z_f^* < \sum_t \Big(\sum_{v \in V} (\hat{p}_v + f_v + k) Q_{tv} \hat{x}_{tv} + \sum_{v \in \bar{V}} (q_v + \bar{f}_v + k) \bar{Q}_{tv} \hat{y}_{tv} \Big)$ **then**

Go to **Step 3**.

end if

Step 3. Add a constraint of the form:
$\sum_t \Big(\sum_{v \in V} (p_v + f_v + k) Q_{tv} x_{tv} + \sum_{v \in \bar{V}} (q_v + \bar{f}_v + k) \bar{Q}_{tv} y_{tv} \Big) \leq \sum_t \Big(\sum_{v \in V} (p_v + f_v + k) Q_{tv} \check{x}_{tv} + \sum_{v \in \bar{V}} (q_v + \bar{f}_v + k) \bar{Q}_{tv} \check{y}_{tv} \Big)$ to **SPVPP** and go to **Step 1**.

5.3.2 Robust PVPP

Next, we extend the developed exact solution approach to robust models $\mathbf{R}^{\mathrm{I}}$**-PVPP** and $\mathbf{R}^{\mathrm{II}}$**-PVPP**. Note that both of these problems can be viewed as three-level problems and, thus, Algorithm 3 cannot be simply employed as a solution method. Therefore, to apply Algorithm 3 for solving these robust problems, we first need to reformulate them as bilevel programs. This can be done by using the KKT optimality conditions or the strong duality property of linear programs, recall our discussion in Chapter 4. Thus, we reformulate $\mathbf{R}^{\mathrm{I}}$**-PVPP** and $\mathbf{R}^{\mathrm{II}}$**-PVPP** as bilevel mixed-integer programs and then apply Algorithm 3 as a solution method. Consider the inner bilevel problem in $\mathbf{R}^{\mathrm{I}}$**-PVPP** for a fixed upper-level variable $\mathbf{p}$:

$$\min_{\mathbf{q}} \sum_t \sum_{v \in V} (p_v - c_v) Q_{tv} x_{tv} \tag{5.5a}$$

$$\text{subject to} \quad 0 \leq q_v - \bar{p}_v \leq \delta_v \qquad \forall v \in \bar{V}, \tag{5.5b}$$

$$\sum_{v \in \bar{V}} (q_v - \bar{p}_v) \leq \Delta, \tag{5.5c}$$

$$\mathbf{x}, \mathbf{y} \in \mathcal{R}(\mathbf{p}, \mathbf{q})$$

Because no discrete variable appears in constraints (5.5b)-(5.5c), we can replace the problem (5.5a)-(5.5c) by its optimality conditions, i.e., the KKT optimality conditions or the strong duality property. Consequently, the three-level problem **R^I-PVPP** reduces to a bilevel reformulation. In particular, the KKT optimality conditions of problem (5.5) is as follows:

$$q_v \geq \bar{p}_v \qquad \forall v \in \bar{V}, \tag{5.6a}$$

$$q_v \leq \bar{p}_v + \delta_v \qquad \forall v \in \bar{V}, \tag{5.6b}$$

$$\sum_{v \in \bar{V}} q_v \leq \Delta + \sum_{v \in \bar{V}} \bar{p}_v, \tag{5.6c}$$

$$\pi_v - \theta_v - \lambda \leq 0 \qquad \forall v \in \bar{V}, \tag{5.6d}$$

$$(q_v - \bar{p}_v)\pi_v = 0 \qquad \forall v \in \bar{V}, \tag{5.6e}$$

$$(\bar{p}_v + \delta_v - q_v)\theta_v = 0 \qquad \forall v \in \bar{V}, \tag{5.6f}$$

$$(\Delta + \sum_{v \in \bar{V}} (\bar{p}_v - q_v))\lambda = 0, \tag{5.6g}$$

$$(\theta_v + \lambda - \pi_v) q_v = 0 \qquad \forall v \in \bar{V}, \tag{5.6h}$$

$$\pi_v,\ \theta_v, \lambda \geq 0, \tag{5.6i}$$

where $\pi_v,\ \theta_v\ \lambda$ represent the corresponding dual decision variables. We note that, constraints (5.6e)-(5.6h) needs to be transformed to a linear set of constraints. This can be implemented by introducing new binary variables $r_v, s_v, z_v, t \in \{0, 1\}$, for $v \in \bar{V}$, as follows:

$$q_v \leq \bar{p}_v + M_1 r_v \qquad \forall v \in \bar{V}, \tag{5.7a}$$

$$\pi_v \leq M_1(1 - r_v) \qquad \forall v \in \bar{V}, \tag{5.7b}$$

$$q_v \geq \bar{p}_v + \delta_v - \hat{M}_1 s_v \qquad \forall v \in \bar{V}, \tag{5.7c}$$

$$\theta_v \leq \hat{M}_1(1 - s_v) \qquad \forall v \in \bar{V}, \tag{5.7d}$$

$$\sum_{v \in \bar{V}} (q_v - \bar{p}_v) \geq \Delta - \bar{M}_1 t, \tag{5.7e}$$

$$\lambda \leq \bar{M}_1(1 - t), \tag{5.7f}$$

$$\pi_v \geq \theta_v + \lambda - \tilde{M}_1 z_v \qquad \forall v \in \bar{V}, \tag{5.7g}$$

$$q_v \leq \tilde{M}_1(1 - z_v) \qquad \forall v \in \bar{V}, \tag{5.7h}$$

where M_1, $\hat{M}_1$, $\bar{M}_1$ and $\tilde{M}_1$ denote sufficiently large constants. Therefore, problem $\mathbf{R}^{\mathrm{I}}$**-PVPP** can be reformulated as the following mixed-integer bilevel program:

$$\begin{aligned}
\max_{\mathbf{p}\in\mathbb{R}_+^{|V|}} \quad & f_1(\mathbf{p},\mathbf{x}) = \sum_t \sum_{v\in V} (p_v - c_v) Q_{tv} x_{tv} \\
\text{subject to} \quad & (5.6a) - (5.6d) \\
& (5.7a) - (5.7h) \\
& q_v, \pi_v,\ \theta_v,\ \lambda \in \mathbb{R}_+,\ r_v,\ s_v,\ z_v,\ t \in \{0,1\}, \\
& \mathbf{x},\mathbf{y} \in \mathcal{R}(\mathbf{p},\mathbf{q})
\end{aligned}$$

Because of the existence of nonlinear terms $p_v x_{tv}$ and $q_v y_{tv}$ this problem is nonlinear. The linearization technique, proposed in this section, can be used to replace these nonlinear terms by variables u_{tv} and w_{tv}, respectively.

We could alternatively replace problem (5.5a)-(5.5c) by applying the strong duality property. In this case, $\mathbf{R}^{\mathrm{I}}$**-PVPP** is equivalent to the following mixed-integer bilevel program:

$$\begin{aligned}
\max_{\mathbf{p}\in\mathbb{R}_+^{|V|}} \quad & f_1(\mathbf{p},\mathbf{x}) = \sum_t \sum_{v\in V} (p_v - c_v) Q_{tv} x_{tv} \\
\text{subject to} \quad & (5.6a) - (5.6d) \\
& \sum_{v\in\bar{V}} \bar{p}_v \pi_v - \sum_{v\in\bar{V}} (\bar{p}_v + \delta_v)\theta_v - (\Delta + \sum_{v\in\bar{V}} \bar{p}_v)\lambda = \sum_t \sum_{v\in V} (p_v - c_v) Q_{tv} x_{tv}, \qquad (5.9a) \\
& q_v, \pi_v,\ \theta_v, \in \mathbb{R}_+^{|\bar{V}|},\ \lambda \in \mathbb{R}_+, \\
& \mathbf{x},\mathbf{y} \in \mathcal{R}(\mathbf{p},\mathbf{q}),
\end{aligned}$$

where constraint (5.9a) represents the strong duality property of problem (5.5a)-(5.5c). Therefore, $\mathbf{R}^{\mathrm{I}}$**-PVPP** can be reformulated as a mixed-integer bilevel program by applying the KKT optimality conditions or the strong duality property.

The same idea can be exploited to reformulate robust problem $\mathbf{R}^{\mathrm{II}}$**-PVPP** as a mixed-integer bilevel problem. That is, by applying either the KKT optimality conditions or the strong duality property, the three-level robust problem $\mathbf{R}^{\mathrm{II}}$**-PVPP** can be reformulated as a mixed-integer bilevel problem. For instance, by applying the strong duality property, we achieve the following mixed-integer bilevel reformulation of $\mathbf{R}^{\text{II}}$-**PVPP**:

$$
\begin{aligned}
\max_{\mathbf{p}\in\mathbb{R}_+^{|V|}} \quad & f_2(\mathbf{p},\mathbf{x}) = \sum_t \sum_{v\in V} (p_v - c_v) Q_{tv} x_{tv} \\
\text{subject to} \quad & q_v \geq \bar{p}_v && \forall v \in \bar{V}, && (5.10a)\\
& q_v \leq \bar{p}_v + \delta_v z_v && \forall v \in \bar{V}, && (5.10b)\\
& \sum_{v\in\bar{V}} z_v \leq \Gamma, && && (5.10c)\\
& \pi_v - \theta_v \leq 0 && \forall v \in \bar{V}, && (5.10d)\\
& \delta_v \theta_v - \lambda \leq 0 && \forall v \in \bar{V}, && (5.10e)\\
& \sum_{v\in\bar{V}} \bar{p}_v \pi_v - \sum_{v\in\bar{V}} \bar{p}_v \theta_v - \Gamma\lambda = \sum_t \sum_{v\in V} (p_v - c_v) Q_{tv} x_{tv}, && && (5.10f)\\
& q_v, \pi_v,\ \theta_v, \in \mathbb{R}_+^{|\bar{V}|},\ \lambda \in \mathbb{R}_+,\ z_v \in [0,1], \\
& \mathbf{x}, \mathbf{y} \in \mathcal{R}(\mathbf{p}, \mathbf{q})
\end{aligned}
$$

Thus, both three-level robust problems $\mathbf{R}^{\text{I}}$-**PVPP** and $\mathbf{R}^{\text{II}}$-**PVPP** can be reformulated as mixed-integer bilevel problems. This transformation enables us to exploit the idea of Algorithm 3 and propose an exact solution approach for these problems. With this approach, in order to solve $\mathbf{R}^{\text{I}}$-**PVPP** and $\mathbf{R}^{\text{II}}$-**PVPP**, we first reformulate them as a mixed-integer bilevel problem. Then, we apply a modified version of Algorithm 3 where instead of solving **SPVPP** in the first step, we solve single-level relaxation of $\mathbf{R}^{\text{I}}$-**PVPP** or $\mathbf{R}^{\text{II}}$-**PVPP**. Proposition 24 assures that these robust formulations can be solved exactly after a limited number of iterations.

5.4 NUMERICAL EXPERIMENTS

In this section we describe our computational experiments aimed at exploring the numerical performance of Algorithm 3 and the reformulations from Section 5.2. We employ the same set of test instances used in [96] where each of three major pediatric vaccine manufacturers in the United States market, GlaxoSmithKline, Merck and Sanofi Pasteur, act as the leader. In addition, the 2014 Recommended Childhood Immunization Schedule (RCIS) [35] and 2014 private sector market prices [36] are used in this set of instances. Similar to [96], the time periods of interest in our study includes: birth, 2-month, 4-month, 6-month, 12-18 months and 4-6 years.

Our experiments are conducted on an Intel Xenon PC with 3.7 GHz CPU and 32 GB of RAM, and MIPs are solved using CPLEX 12.4 [67]. As reported in [96], the heuristic methods of [96] are coded in C++ and the lower-level problem, for any set of p_v-variables, is solved using CPLEX 12.5. All runs in [96] are implemented on a PC having an AMD Athlon II X2 215 processor with 2.7 GHz CPU and 4 GB of RAM.

Running time analysis. First, in Table 17, we study the performance of Algorithm 3 in terms of its running time. Three forms of heuristic algorithm, denoted by H1, H2 and H3, are developed in [96] to solve **DPVPP**. In each of these heuristic methods, the value of parameter ψ represents the number of selected points for the p_v-variables within a given sampling region. We apply Algorithm 3 to solve the same set of test instances used in [96] to compare its running time against the reported running time of the best three variants of heuristic methods developed in [96].

Table 17 demonstrates that, although these three heuristic methods are not guaranteed to achieve an optimal solution, they result in relatively good pricing decisions. In particular, the third heuristic variant, $\psi = 1000$, obtains an optimal solution in all test instances. This can be observed by comparing the manufacturer's profit obtained by the heuristic methods against the optimal profit obtained by exact Algorithm 3.

However, from the running time point of view, these heuristic methods are slower than Algorithm 3. Indeed, Algorithm 3 reaches an optimal solution, in all test instances, significantly faster than the heuristic approaches, see the bolded values in Table 17.

Note that, as the gap between the profit from the heuristic methods and the optimal profit in Algorithm 3 decreases, the running time of these heuristic algorithms increases. That is, the best heuristic method in [96], in terms of reaching a good solution, $\psi = 1000$, is the slowest one. However, Algorithm 3 reaches an optimal solution quickly, see, Section 5.3.

Table 17: The running times (in seconds) of solving **DPVPP** instances, by three variants of the heuristic methods developed in [96] and Algorithm 3. The running times of heuristic methods are taken from [96] for each row. The value in **bold** represents the best result across all methods. The value in parenthesis shows the number of iterations in Algorithm 3.

Manufacturer	k ($)		Heuristic H3			Algorithm 3
			$\psi = 10$	$\psi = 100$	$\psi = 1000$	
GlaxoSmithKline	6.79	profit	264.32	298.44	298.44	298.44
		time	32	375	4340	**2** (10)
	9.31	profit	298.44	298.44	298.44	298.44
		time	30	543	3559	**3** (10)
	11.83	profit	298.44	298.44	298.44	298.44
		time	30	243	3100	**4** (11)
	14.35	profit	298.44	302.47	302.47	302.47
		time	27	332	3277	**3** (11)
	16.87	profit	298.44	312.55	312.55	312.55
		time	32	326	2105	**3** (10)
Merck	6.79	profit	93.7	93.7	93.7	93.7
		time	15	137	1250	**3** (5)
	9.31	profit	93.7	93.7	93.7	93.7
		time	14	131	1945	**3** (5)
	11.83	profit	93.7	93.7	93.7	93.7
		time	11	142	1260	**2** (5)
	14.35	profit	83.7	93.7	93.7	93.7
		time	13	146	1399	**2** (4)
	16.87	profit	93.7	93.7	93.7	93.7
		time	13	136	1431	**2** (4)
Sanofi Pasteur	6.79	profit	220.6	245.1	251.04	251.04
		time	30	261	2432	**3** (7)
	9.31	profit	220.6	238.39	248.52	248.52
		time	97	278	3488	**3** (7)
	11.83	profit	220.6	238.39	246	246
		time	23	254	2715	**2** (7)
	14.35	profit	220.6	238.39	243.48	243.48
		time	23	273	2529	**3** (7)
	16.87	profit	220.6	239.39	240.96	240.96
		time	23	270	2590	**3** (7)

Comparing robust formulations and DPVPP. To study the advantages and limitations of proposed robust models in different situations, in this set of experiments we provide a detailed comparison between these models and **DPVPP**. We consider the manufacturer's profit in different settings where the value of q_v is known, for all vaccines $v \in \bar{V}$, or is given by uncertainty sets Ω_1 or Ω_2. For each setting, we explore the obtained profit when the manufacturer implements a robust solution or an optimal solution of **DPVPP**. Throughout our experiments, the values of parameter $\bar{p}_v$, in robust models, and q_v, in **DPVPP**, are set to the market prices used in [96] for all vaccines $v \in \bar{V}$.

In Table 18 we evaluate the manufactures' profit in a nondeterministic setting where the value of q_v, for all vaccines $v \in \bar{V}$, is given by the uncertainty set Ω_1 with $\Delta = 20$ and $\delta_v = 8$. Let $(\mathbf{p}_1^*, \mathbf{x}_1^*)$ be the optimal solution of $\mathbf{R}^{\mathrm{I}}$**-PVPP**. Then, we denote by $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$, the corresponding optimal objective function value of $\mathbf{R}^{\mathrm{I}}$**-PVPP**. Furthermore, we report the profit obtained when the manufacturer ignores the uncertainty in the market prices and implements an optimal solution of **DPVPP**, denoted by $\mathbf{p}_d^*$, see the values of $f_1(\mathbf{p}_d^*, \mathbf{x}_d)$ in Table 18, where $\mathbf{x}_d$ is the lower-level response to the upper-level decision $\mathbf{p}_d^*$. Thus, $f_1(\mathbf{p}_d^*, \mathbf{x}_d)$ is the manufacturer's objective function value if upper-level decision $\mathbf{p}_d^*$ is plugged into problem $\mathbf{R}^{\mathrm{I}}$**-PVPP**.

The optimal objective function value of $\mathbf{R}^{\mathrm{I}}$**-PVPP**, $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$, in Table 18, shows the manufacturer's worst profit if she/he takes the uncertainty into consideration and sets the vaccines prices through solving $\mathbf{R}^{\mathrm{I}}$**-PVPP**. If the manufacturer implements solution $\mathbf{p}_d^*$, which is not necessarily an optimal decision in this nondeterministic setting, then the obtained profit is smaller, see the values of $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$ and $f_1(\mathbf{p}_d^*, \mathbf{x}_d)$ in Table 18. The value of the profit reduction is reported for all instances in Table 18. For example, in the first two instances, if the manufacturer implements $\mathbf{p}_d^*$, then the resulting profit can be zero in the worst case. However, in these two instances, if an optimal solution of $\mathbf{R}^{\mathrm{I}}$**-PVPP** is implemented, then the profit is at least 90.09 and 62.66, respectively.

Table 19 displays the manufactures' profit in a different setting where the value of q_v is known for all vaccines $v \in \bar{V}$. The profit is reported when the manufacturer makes use of extra information about market prices and sets the prices through solving deterministic model **DPVPP**, see $f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$. Moreover, we compute the profit if the manufacturer implements

Table 18: Obtained profit in a nondeterministic setting when the manufacturer implements either an optimal solution of $\mathbf{R^I}$**-PVPP** or **DPVPP**. An optimal solution of $\mathbf{R^I}$**-PVPP** is denoted by $(\mathbf{p}_1^*, \mathbf{x}_1^*)$ and $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$ is the corresponding optimal objective function value. The value of $\mathbf{p}_d^*$ represents an optimal solution of **DPVPP** and $f_1(\mathbf{p}_d^*, \mathbf{x}_d)$ is the objective function value of $\mathbf{R^I}$**-PVPP** when the manufacturer implements $\mathbf{p}_d^*$. We set $\Delta = 20$ and $\delta_v = 8$, for all vaccines $v \in \bar{V}$.

Manufacturer	k	$f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$	$f_1(\mathbf{p}_d^*, \mathbf{x}_d)$	$f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$ $-f_1(\mathbf{p}_d^*, \mathbf{x}_d)$	$\frac{f_1^*(\mathbf{p}_1^*,\mathbf{x}_1^*)-f_1(\mathbf{p}_d^*,\mathbf{x}_d)}{f_1^*(\mathbf{p}_1^*,\mathbf{x}_1^*)} \times 100\%$
GlaxoSmithKline	6.79	90.09	0	90.09	100
	9.31	62.66	0	62.66	100
	11.83	90.09	66.76	23.33	26
	14.35	127.94	66.76	61.18	48
	16.87	132.98	66.76	66.22	50
Merck	6.79	78.83	68.77	10.06	13
	9.31	65.52	57.76	7.76	12
	11.83	65.52	57.76	7.76	12
	14.35	65.52	57.76	7.76	12
	16.87	65.52	57.76	7.76	12
Sanofi Pasteur	6.79	61.05	17.57	43.48	71
	9.31	23.05	15.05	8.00	35
	11.83	20.05	12.53	7.52	38
	14.35	53.59	10.01	43.58	81
	16.87	36.29	7.49	28.80	79

an optimal decision of $\mathbf{R^I}$**-PVPP**, denoted by $\mathbf{p}_1^*$, in this deterministic setting, see $f_d(\mathbf{p}_1^*, \mathbf{x}_1)$. As expected, compared with the value of $f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$, the resulting profit in the second case is smaller. We can interpret this difference in Table 19 as "the value of information" for manufacturers in an oligopolistic vaccine market.

By applying robust model $\mathbf{R^I}$**-PVPP** in a nondeterministic setting, a manufacturer considers the worst-case scenarios with respect to the value of q_v, see $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$ in Table 18. That is, for any set of $q_v \in \Omega_1$, the manufacturer's profit is equal to or greater than the value of $f_1^*(\mathbf{p}_1^*, \mathbf{x}_1^*)$. This can be observed through comparing the values $(\mathbf{p}_1^*, \mathbf{x}_1^*)$ in Tables 18 with $f_d^*(\mathbf{p}_1^*, \mathbf{x}_1)$ in Table 19 where the values of q_v are fixed for all vaccines $v \in \bar{V}$.

Tables 20 and 21 present similar information where the manufacturers apply model $\mathbf{R}^{\mathrm{II}}$-**PVPP** to achieve a robust pricing decision. The corresponding uncertainty set in $\mathbf{R}^{\mathrm{II}}$-**PVPP** is represented by Ω_2 where $\Gamma = 2$ and $\delta_v = 8$, for all vaccines $v \in \bar{V}$.

Table 19: Obtained profit in a deterministic setting when the manufacturer implements either an optimal solution of **DPVPP** or $\mathbf{R}^{\mathrm{I}}$-**PVPP**. An optimal solution of **DPVPP** is denoted by $(\mathbf{p}_d^*, \mathbf{x}_d^*)$ and $f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$ represents the corresponding optimal objective function value. The value of $\mathbf{p}_1^*$ represents an optimal solution of $\mathbf{R}^{\mathrm{I}}$-**PVPP** and $f_d(\mathbf{p}_1^*, \mathbf{x}_1)$ is the objective function value of **DPVPP** when the manufacturer implements $\mathbf{p}_1^*$. We set $\Delta = 20$ and $\delta_v = 8$, for all vaccines $v \in \bar{V}$.

Manufacturer	k	$f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$	$f_d(\mathbf{p}_1^*, \mathbf{x}_1)$	$f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$ $-f_d(\mathbf{p}_1^*, \mathbf{p}_1)$	$\frac{f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*) - f_d(\mathbf{p}_1^*, \mathbf{p}_1)}{f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)} \times 100\%$
GlaxoSmithKline	6.79	298.47	90.09	208.38	70
	9.31	298.47	149.57	148.90	50
	11.83	298.47	155.57	142.90	48
	14.35	302.47	181.26	121.21	40
	16.87	312.594	245.54	67.05	21
Merck	6.79	93.7	78.83	14.87	16
	9.31	93.7	65.52	28.18	30
	11.83	93.7	65.52	28.18	30
	14.35	93.7	65.52	28.18	30
	16.87	93.7	65.52	28.18	30
Sanofi Pasteur	6.79	251.057	61.15	189.90	76
	9.31	248.537	58.63	189.90	76
	11.83	246.017	56.11	189.90	77
	14.35	243.317	53.59	189.72	78
	16.87	240.977	53.59	187.387	78

Table 20: Obtained profit in a nondeterministic setting when the manufacturer implements either an optimal solution of $\mathbf{R}^{\text{II}}$**-PVPP** or **DPVPP**. An optimal solution of $\mathbf{R}^{\text{II}}$**-PVPP** is denoted by $(\mathbf{p}_2^*, \mathbf{x}_2^*)$ and $f_2^*(\mathbf{p}_2^*, \mathbf{x}_2^*)$ is the corresponding optimal objective function value. The value of $\mathbf{p}_d^*$ represents an optimal solution of **DPVPP** and $f_2(\mathbf{p}_d^*, \mathbf{x}_d)$ is the objective function value of $\mathbf{R}^{\text{II}}$**-PVPP** when the manufacturer implements $\mathbf{p}_d^*$. We set $\Delta = 20$ and $\delta_v = 8$, for all vaccines $v \in \bar{V}$.

Manufacturer	k	$f_2^*(\mathbf{p}_2^*, \mathbf{x}_2^*)$	$f_2(\mathbf{p}_d^*, \mathbf{x}_d)$	$f_2^*(\mathbf{p}_2^*, \mathbf{x}_2^*)$ $-f_2(\mathbf{p}_d^*, \mathbf{x}_d)$	$\frac{f_2^*(\mathbf{p}_2^*,\mathbf{x}_2^*)-f_2(\mathbf{p}_d^*,\mathbf{x}_d)}{f_2^*(\mathbf{p}_2^*,\mathbf{x}_2^*)} \times 100\%$
GlaxoSmithKline	6.79	144.82	90.92	53.90	37
	9.31	98.92	90.92	8.00	8
	11.83	98.92	90.92	8.00	8
	14.35	127.94	66.76	61.18	48
	16.87	180.62	132.98	47.64	26
Merck	6.79	74.84	49.53	25.31	34
	9.31	65.53	49.53	16.00	25
	11.83	65.53	49.53	16.00	25
	14.35	65.53	49.53	16.00	25
	16.87	65.53	49.53	16.00	25
Sanofi Pasteur	6.79	25.59	17.57	8.02	31
	9.31	23.05	15.05	8.00	35
	11.83	17.79	12.53	5.26	29
	14.35	17.79	10.53	7.26	40
	16.87	17.79	15.09	2.70	15

Table 21: Obtained profit in a deterministic setting when the manufacturer implements either an optimal solution of **DPVPP** or $\mathbf{R}^{\mathrm{II}}$-**PVPP**. An optimal solution of **DPVPP** is denoted by $(\mathbf{p}_d^*, \mathbf{x}_d^*)$ and $f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$ represents the corresponding optimal objective function value. The value of $\mathbf{p}_2^*$ represents an optimal solution of $\mathbf{R}^{\mathrm{II}}$-**PVPP** and $f_d(\mathbf{p}_2^*, \mathbf{x}_2)$ is the objective function value of **DPVPP** when the manufacturer implements $\mathbf{p}_2^*$. We set $\Delta = 20$ and $\delta_v = 8$, for all vaccines $v \in \bar{V}$.

Manufacturer	k	$f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$	$f_d(\mathbf{p}_2^*, \mathbf{x}_2)$	$f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)$ $-f_d(\mathbf{p}_2^*, \mathbf{p}_2)$	$\frac{f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*) - f_d(\mathbf{p}_2^*, \mathbf{p}_2)}{f_d^*(\mathbf{p}_d^*, \mathbf{x}_d^*)} \times 100\%$
GlaxoSmithKline	6.79	298.47	167.07	131.40	44
	9.31	298.47	171.07	127.40	43
	11.83	298.47	175.07	123.40	41
	14.35	302.47	177.07	125.40	41
	16.87	312.59	181.07	131.52	42
Merck	6.79	93.70	74.84	18.86	20
	9.31	93.70	65.52	28.18	30
	11.83	93.70	65.52	28.18	30
	14.35	93.70	65.52	28.18	30
	16.87	93.70	65.52	28.18	30
Sanofi Pasteur	6.79	251.05	61.15	189.90	76
	9.31	248.53	58.63	190.38	76
	11.83	246.01	17.79	228.22	93
	14.35	243.31	17.79	225.52	93
	16.87	240.97	17.79	223.18	93

5.5 CONCLUSION

In this chapter we consider the pediatric vaccine pricing problem in the US oligopolistic market. We formulate this problem as a mixed-integer nonlinear bilevel program, where at the upper level the manufacturer sets the vaccine price and at the lower level, a potential purchaser, e.g., a health care provider, seeks to minimize the cost of vaccination. That is, the purchaser has to decide whether to purchase a vaccine from the manufacturer or from the other producers in the market, i.e., competitors.

In contrast to the previous works in the literature, see [96], we study this problem in a nondeterministic setting, where the price of vaccines produced by the competitors are given by some uncertainty sets. Specifically, we extend [96] by proposing different robust formulations for situations where the market prices of vaccines are not known exactly in advance. Furthermore, we develop an exact solution method for the presented formulations.

For future research, it would be valuable to develop a model that takes into account both private and public market prices. Another interesting direction includes extending this model to incorporate settings, where different financial incentives for manufacturers are provided by the government. Furthermore, it would be beneficial to consider this problem in settings where vaccine prices are given by different types of uncertainty sets.

6.0 CONCLUSION

One of the key assumptions in the standard bilevel optimization modeling framework is that the follower solves the lower-level problem optimally. However, there are many practical application settings where this assumption is not likely to hold. In this dissertation we address this issue by proposing different modeling approaches where the follower's reaction set includes exact and inexact solutions of the lower-level problem. Moreover, we develop solution methods to solve the proposed bilevel models and demonstrate their performance through extensive numerical experiments.

Chapter 2 considers a general class of pessimistic bilevel linear problems, referred to as α-pessimistic BMIPs, where the follower might select a suboptimal solution, to worsen the leader's situation. We incorporate the proposed approach into a class of strong-weak models, where the leader is not certain if the follower is either collaborative or adversarial. The advantages and limitations of the proposed approaches are illustrated by using insightful numerical experiments. Moreover, we consider some related computational complexity issues. In particular, the most interesting observation obtained is the fact that even if an optimal optimistic (or pessimistic) solution of BLP is known, then the problem of finding an optimal pessimistic (or optimistic) solution for the same BLP remains an NP-hard problem. Future research directions may include issues related to generalizations of the proposed models for bilevel problems that involve integrality restrictions for the follower's decision variables and more general classes of objective functions at both levels.

Chapter 3 considers different modeling approaches for situations where the leader does not know upfront the algorithm used by the follower to solve the lower-level problem, but knows that it belongs to a known finite set of algorithms. Three approaches are proposed that allow the leader to hedge against different response scenarios at the lower level. Our results indicate that the proposed approaches allow the leader to substantially reduce her losses whenever the follower's actual behavior is not known precisely. An interesting future extension of our work may include settings where the leader and the follower interact repeatedly over time, and hence the leader might infer information regarding the method used by the follower based on his response to the leader decisions.

Chapter 4 studies single-level reformulations of bilevel problems, including those presented in Chapters 2 and 3. We propose a new reformulation method for this reformulation based on the strong duality property of linear optimization problems under the assumption that the upper-level variables are integer. Compared to the KKT-based reformulation, SD-based reformulation may reduce the number of variables and constraints significantly in some settings. We perform extensive numerical experiments to explore the performances of an off-the-shelf MIP solver with these reformulations. Our experiments show that the SD-based reformulations can lead to orders of magnitude reduction in computational times for certain classes of problems.

Chapter 5 explores bilevel models in the application setting of the pediatric vaccine pricing problem. We present different robust bilevel formulations of this problem, assuming that the competitors' prices are nondeterministic. Moreover, we develop an iterative exact solution method where the MIP single-level relaxation models are solved in each iteration. Our numerical results demonstrate that compared to the existing approaches in the literature, our robust models may improve the manufacturer's profit.

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