Easier than We Thought – A Practical Scheme to Compute Pessimistic Bilevel Optimization Problem

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Abstract

In this paper, we present a new computation scheme for pessimistic bilevel optimization problem, which so far does not have any computational methods generally applicable yet. We first develop a tight relaxation and then design a simple scheme to ensure a feasible and optimal solution. Then, we discuss using this scheme to compute linear pessimistic bilevel problem and several variants. We also provide numerical demonstrations on instances of those linear pessimistic bilevel problems. Because of its simplicity and convenient interfaces to existing algorithms of the regular (optimistic) bilevel problem, we believe that the developed scheme is of a great significance in solving pessimistic bilevel optimization problems arising from various practical systems.

1 Background

Bilevel optimization is a popular modeling and computing tool for non-centralized decision making problems where two decision makers (DMs), i.e., the upper level and the lower level DMs, interact sequentially. In this paper, we consider the *pessimistic formulation* (also known as the *weak formulation*) of bilevel optimization [23], which can be represented in the following mathematical form:

$$\mathbf{PBL}: \quad \Theta_p^* = \min_{\mathbf{x} \in \mathbb{X}} \ \max_{\mathbf{y} \in \mathbf{S}(\mathbf{x})} \ \mathbf{F}(\mathbf{x}, \mathbf{y}) \tag{1}$$

$$\text{s.t.} \quad \mathbf{G}(\mathbf{x}) \leq \mathbf{0} \tag{2}$$

$$\mathbf{S}(\mathbf{x}) = \arg\min \left\{ \mathbf{f}(\mathbf{x}, \mathbf{y}) : \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}, \mathbf{y} \in \mathbb{Y} \right\} \tag{3}$$

where $\mathbb{X} \subseteq \mathbb{R}^n$ and $\mathbb{Y} \subseteq \mathbb{R}^m$. We mention that neither $\mathbb{X}$ nor $\mathbb{Y}$ is required to be a continuous set, i.e., $\mathbf{x}$ or $\mathbf{y}$ could be discrete variables. The optimization problem defined in (1-2) is referred to as the upper level DM's (her) decision problem and the one appearing in (3) is called the lower level DM's (his) decision problem. Hence, $\mathbf{S}(\mathbf{x})$ represents the collection of optimal solutions of the lower level problem for a given $\mathbf{x}$.

Note that if we simply drop the *max* operation in (1), i.e.,

$$\min_{\mathbf{x} \in \mathbb{X}} \max_{\mathbf{y} \in \mathbf{S}(\mathbf{x})} \mathbf{F}(\mathbf{x}, \mathbf{y}) \;\Rightarrow\; \min_{\mathbf{x} \in \mathbb{X}, \mathbf{y} \in \mathbf{S}(\mathbf{x})} \mathbf{F}(\mathbf{x}, \mathbf{y}),$$

the formulation in (1-3) reduces to the regular *optimistic formulation* (also known as the *strong formulation*). We use **OBL** and Θ_o^* to denote the latter one and its optimal value, respectively. Clearly, if $\mathbf{S}(\mathbf{x})$ is a singleton for every $\mathbf{x}$, those two formulations are identical. However, $\mathbf{S}(\mathbf{x})$ might be a set with multiple elements, which is often observed in a few decomposition algorithms for bilevel optimization problems [24, 30]. Given that, if the lower level DM is believed to be cooperative by always selecting a solution from $\mathbf{S}(\mathbf{x})$ in favor of the upper level DM, we can adopt the optimistic formulation. Nevertheless, if the lower level DM behaves non-cooperatively by taking a solution against the upper level DM's interest, we should employ the pessimistic formulation for modeling and computing.

The origin of bilevel optimization can be linked to the development of Stackelberg leader-follower game [28] on the investigation of market equilibrium in 1930s. Its first explicit mathematical formulation can be found in [7] in 1970s. Over the last 40 years, there is a great amount of research developed on bilevel optimization [17, 5, 14]. Theoretically, it is recognized that computing a bilevel optimization problem is not easy. Even for (optimistic) bilevel linear programming (LP) problem where both upper and lower level problems are LPs, it is NP-hard [19, 4]. To address such challenge, many computational strategies and algorithms have been proposed, developed and investigated (see [17, 5, 14, 30] and references therein), the vast majority of which, however, is devoted to solving the optimistic formulation. As a result, those advanced and capable computing tools strongly support the real applications of optimistic bilevel models in transportation planning and capacity expansion [8, 25], government policy making [6, 13], revenue management [9, 15], electricity market [21, 20] and computational biology [26, 10].

On the contrary, the pessimistic model is thought to be much more difficult than the optimistic one, and we generally believe that the solution methodologies developed for the latter one cannot be directly applied. Up to now, the pessimistic bilevel problem only receives a very limited amount of attention. One way to attack it is to compute a sequence of optimistic bilevel models that include a penalty term on the upper level objective value in the lower level objective function [23, 3]. Similarly, when **PBL** is pure linear [2], it can be solved by a sequence bilinear programs that penalize the difference between the primal and dual of lower level problem. Recently, one type of bilevel problem with coupled pessimistic constraints, i.e., constraints must be satisfied by the selected $\mathbf{x}$ and all solutions in $\mathbf{S}(\mathbf{x})$, is studied in [27, 29]. Authors argue that it generalizes the regular pessimistic bilevel model presented in (1-3). In a special case where the feasible set of the lower level problem has nothing to do with the upper level variable $\mathbf{x}$, which is referred to as the independent **PBL**, they propose an ϵ-approximation of **PBL** to ensure the existence of an optimal solution and develop an iterative procedure using semi-infinite programming techniques to compute that ϵ-approximation. We note, however, that all the aforementioned iterative methods require a global solution at every update, even for the simplest linear **PBL**. So, they do not render themselves to practical **PBL** instances.

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It is worth mentioning that in [18, 16], various necessary optimality conditions for continuous **PBL** are derived, which could be helpful to develop fast algorithms to compute (local) optimal solutions.

In this paper, we mainly focus on developing a new computing scheme for **PBL** formulation that has an optimal solution. Specifically, in Section 2, we develop a regular bilevel formulation that is a tight relaxation to the general **PBL** and present a two-step computing scheme to derive a feasible and optimal solution for **PBL**. In Section 3, we then discuss using this scheme to compute linear **PBL** and its several variants. In Section 4, we provide numerical demonstrations on instances of those linear **PBL** problems. Section 5 concludes this paper. We would like to highlight that, because this method allows us to fully take advantage of existing research on regular bilevel problems and does not involve any sophisticated theory or operations, it is very friendly and convenient to support practitioners to address real challenges in various applications.

2 A New Scheme for Level Reduction and Computation

Let $\mathbf{X} = \{\mathbf{x} \in \mathbb{X} : \mathbf{G}(\mathbf{x}) \leq \mathbf{0}\}$ and $\mathbf{Y}(\mathbf{x}) = \{\mathbf{y} \in \mathbb{Y} : \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}\}$ for $\mathbf{x} \in \mathbf{X}$. In this section, we make two rather standard assumptions: (a) function $\mathbf{f}$ is continuous over its domain and (b) $\mathbf{Y}(\mathbf{x})$ is compact for $\mathbf{x} \in \mathbf{X}$. Those two assumptions ensure that for a given $\mathbf{x}$, the lower level problem is either infeasible or has an optimal solution.

2.1 A Tight Relaxation for Level Reduction

Pessimistic bilevel problem is generally formulated as a three level problem, as in (1-3). Apparently, it is more complicated than its bilevel optimistic counterpart **OBL**. Indeed, it is easy to see that **OBL** is a relaxation and its optimal value provides a lower bound to **PBL**. Because such relaxation is straightforward, we would say it is trivial. In the following, by introducing a set of variables and constraints that replicate those in the lower level, we present a non-trivial bilevel relaxation.

Lemma 1. *The following formulation R-PBL is a relaxation to PBL.*

$$\textbf{\textit{R-PBL}}: \quad \tilde{\Theta}_p^* = \min_{\mathbf{x}, \overline{\mathbf{y}}} \ \max_{\mathbf{y} \in \tilde{\mathbf{Y}}(\mathbf{x}, \overline{\mathbf{y}})} \ \mathbf{F}(\mathbf{x}, \mathbf{y}) \tag{4}$$

$$s.t. \quad \mathbf{G}(\mathbf{x}) \leq \mathbf{0}, \ \mathbf{x} \in \mathbb{X}, \tag{5}$$

$$\mathbf{g}(\mathbf{x}, \overline{\mathbf{y}}) \leq \mathbf{0}, \ \overline{\mathbf{y}} \in \mathbb{Y}, \tag{6}$$

$$\tilde{\mathbf{Y}}(\mathbf{x}, \overline{\mathbf{y}}) = \left\{ \mathbf{y} \in \mathbb{Y} : \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}, \mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}, \overline{\mathbf{y}}) \right\} \tag{7}$$

Proof. Consider a fixed $\mathbf{x}^* \in \mathbf{X}$ and $\mathbf{y}^* \in \arg\max\{\mathbf{F}(\mathbf{x}^*, \mathbf{y}) : \mathbf{y} \in \mathbf{S}(\mathbf{x}^*)\}$, i.e., solution $(\mathbf{x}^*, \mathbf{y}^*)$ is feasible to **PBL**. We set $\overline{\mathbf{y}}^* = \mathbf{y}^*$ and extend $(\mathbf{x}^*, \mathbf{y}^*)$ to a 3-tuple $(\mathbf{x}^*, \overline{\mathbf{y}}^*, \mathbf{y}^*)$. It is easy to see that the latter one satisfies constraints in (5-6) and $\mathbf{y}^*$ belongs to $\tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*)$. Moreover, because $\overline{\mathbf{y}}^* = \mathbf{y}^* \in \mathbf{S}(\mathbf{x}^*)$, we have

$$\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*) = \mathbf{f}(\mathbf{x}^*, \mathbf{y}^*) = \min\left\{ \mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{g}(\mathbf{x}^*, \mathbf{y}) \leq \mathbf{0}, \mathbf{y} \in \mathbb{Y} \right\}.$$

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Then, comparing the definitions of $\tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*)$ and $\mathbf{S}(\mathbf{x}^*)$, it is clear that those two sets are identical, i.e., $\tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*) = \mathbf{S}(\mathbf{x}^*)$. Hence, $\mathbf{y}^* \in \arg\max\{\mathbf{F}(\mathbf{x}^*, \mathbf{y}) : \mathbf{y} \in \tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*)\}$. Therefore, the 3-tuple $(\mathbf{x}^*, \overline{\mathbf{y}}^*, \mathbf{y}^*)$ is feasible to **R-PBL**.

Because they share the same objective function, it follows that **R-PBL** is a relaxation to **PBL**. $\qquad\square$

Indeed, it can be proven that this relaxation is tight.

Lemma 2. *For a fixed* $\mathbf{x}^* \in \mathbf{X}$ *such that* $\mathbf{Y}(\mathbf{x}^*)$ *is not empty,* *R-PBL* *has an optimal solution* $(\mathbf{x}^*, \overline{\mathbf{y}}^*, \mathbf{y}^*)$ *such that*

$$\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*) = \min\left\{\mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{g}(\mathbf{x}^*, \mathbf{y}) \leq \mathbf{0}, \mathbf{y} \in \mathbb{Y}\right\}, \tag{8}$$

and $\tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*) = \mathbf{S}(\mathbf{x}^*)$.

Proof. Let $\phi(\mathbf{x}, \overline{\mathbf{y}}) = \max\{\mathbf{F}(\mathbf{x}, \mathbf{y}) : \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}, \mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}, \overline{\mathbf{y}}), \mathbf{y} \in \mathbb{Y}\}$. On the one hand, it is clear that $\phi(\mathbf{x}, \overline{\mathbf{y}})$ is a non-decreasing function with respect to $\mathbf{f}(\mathbf{x}, \overline{\mathbf{y}})$. On the other hand, for $\mathbf{x}^*$, because $\mathbf{f}$ is continuous, $\mathbf{Y}(\mathbf{x}^*)$ is compact, and by Weierstrass theorem, we have that $\min\{\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}) : \mathbf{g}(\mathbf{x}^*, \overline{\mathbf{y}}) \leq \mathbf{0}, \overline{\mathbf{y}} \in \mathbb{Y}\}$ has a minimizer. Let it be denoted by $\overline{\mathbf{y}}^*$. Then, the minimum of $\phi(\mathbf{x}^*, \overline{\mathbf{y}})$ is achieved with the desired properties. $\qquad\square$

Consequently, the next result follows.

Proposition 3. (*i*) *One optimal solution to* *R-PBL* *solves* *PBL*, *and* (*ii*) *among* *OBL*, *PBL* *and* *R-PBL* *formulations, we have* $\Theta_o^* \leq \tilde{\Theta}_p^* = \Theta_p^*$. $\qquad\square$

This result suggests that we probably can compute the three level **PBL** model by investigating a regular bilevel **R-PBL** formulation. It is worth pointing out that such level reduction simply uses the primal representation of the lower level problem, which does not rely on the convexity, strong duality, or Karush-Kuhn-Tucker (KKT) conditions of that problem. So, almost all existing solution methods for regular (optimistic) bilevel problems, including those for discrete or non-convex bilevel problems, can readily be applied to solve **R-PBL** and then to compute **PBL**.

2.2 Computing PBL by R-PBL: A Complete Computational Scheme

Before we proceed to compute **PBL**, it would be worth examining that an optimal solution $(\mathbf{x}^\star, \mathbf{y}^\star)$ obtained for the trivial relaxation **OBL** is not feasible to **PBL**. Otherwise, we can simply report it as an optimal solution to **PBL**. The examination can be done easily by the *lexicographic method* that is often used in multi-objective optimization. Specifically, given that $\mathbf{f}(\mathbf{x}^\star, \mathbf{y}^\star)$ is the optimal lower level value with respect to $\mathbf{x}^\star$, we compute

$$
\begin{aligned}
\max \quad & \mathbf{F}(\mathbf{x}^\star, \mathbf{y}) \\
\text{s.t.} \quad & \mathbf{g}(\mathbf{x}^\star, \mathbf{y}) \leq \mathbf{0}, \ \ \mathbf{f}(\mathbf{x}^\star, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}^\star, \mathbf{y}^\star), \ \mathbf{y} \in \mathbb{Y}.
\end{aligned}
$$

Clearly, if its optimal value is equal to $\mathbf{F}(\mathbf{x}^\star, \mathbf{y}^\star)$, $(\mathbf{x}^\star, \mathbf{y}^\star)$ is feasible and optimal to **PBL** and we do not need to implement any additional operation. Hence, in the remaining part of

this paper, we assume without loss of generality that such examination step is done and it is necessary to compute **PBL** explicitly.

Although **R-PBL** is a tight relaxation, we point out that computing **R-PBL** may not directly generate a feasible solution to **PBL**. It is possible that the solution procedure produces a solution $(\mathbf{x}^*, \overline{\mathbf{y}}^*, \mathbf{y}^*)$ that does not satisfies (8), which indicates that $\mathbf{y}^*$ might not belong to $\mathbf{S}(\mathbf{x}^*)$. For example, when $\mathbf{F}(\mathbf{x}, \mathbf{y}) = 0$, one optimal solution to **R-PBL** can be found with an $\mathbf{x}^*$ and $\overline{\mathbf{y}}^* = \mathbf{y}^* \in \arg\max\{\mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{Y} \in \mathbf{Y}(\mathbf{x}^*)\}$. Whenever $\max\{\mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{Y} \in \mathbf{Y}(\mathbf{x}^*)\} \neq \min\{\mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{Y} \in \mathbf{Y}(\mathbf{x}^*)\}$, that solution is infeasible to **PBL**. Nevertheless, such issue can be easily addressed by the following simple two-step operation, which we refer to as the *Relaxation-and-Correction* computational scheme for **PBL**.

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(1) Relaxation: Compute the tight relaxation **R-PBL** and derive an optimal solution $(\mathbf{x}^*, \overline{\mathbf{y}}^*, \mathbf{y}^*)$. If

$$\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*) > \theta(\mathbf{x}^*) = \min\left\{\mathbf{f}(\mathbf{x}^*, \mathbf{y}) : \mathbf{g}(\mathbf{x}^*, \mathbf{y}) \leq \mathbf{0}, \mathbf{y} \in \mathbb{Y}\right\}, \tag{9}$$

perform the correction step. Otherwise, report $(\mathbf{x}^*, \mathbf{y}^*)$ as an optimal solution to **PBL**.

(2) Correction: Compute

$$\begin{aligned}
\max \quad & \mathbf{F}(\mathbf{x}^*, \mathbf{y}) \\
\text{s.t.} \quad & \mathbf{g}(\mathbf{x}^*, \mathbf{y}) \leq \mathbf{0}, \ \ \mathbf{f}(\mathbf{x}^*, \mathbf{y}) \leq \theta(\mathbf{x}^*), \ \mathbf{y} \in \mathbb{Y}
\end{aligned}$$

and derive an optimal solution $\mathbf{y}'$. Report $(\mathbf{x}^*, \mathbf{y}')$ as an optimal solution to **PBL**. $\quad\square$

According to Lemma 2 and Proposition 3, the correctness of the *Relaxation-and-Correction* scheme is clear. Note that equation (9) is to justify $\tilde{\mathbf{Y}}(\mathbf{x}^*, \overline{\mathbf{y}}^*) = \mathbf{S}(\mathbf{x}^*)$. If not, the lexicographic method is implemented in the correction step. Indeed, we can reduce the occurrence of correction step through replacing $\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*)$ by $\mathbf{f}(\mathbf{x}^*, \mathbf{y}^*)$ in (9).

Within the *Relaxation-and-Correction* scheme, it can be seen that the essential computation of the original three level formulation **PBL** reduces to that of a bilevel problem **R-PBL**. Compared to the optimistic counterpart **OBL**, in particular, the size of **R-PBL** does not increase much. Its lower level problem just has one more constraint than that of the optimistic counterpart, and its upper level problem just has one replica of the lower level variables and constraints. So, solving **R-PBL** does not impose drastically more computational burden.

Another critical observation, as shown in the following, is that the lower level problem in **R-PBL** is often a well-structured optimization problem.

Corollary 4. *If functions $\mathbf{F}$ is concave, $\mathbf{f}$ and $\mathbf{g}$ are convex with respect to $\mathbf{y}$, and $\mathbb{Y}$ is a convex set, the lower level problem in **R-PBL**, i.e.,*

$$\max\left\{\mathbf{F}(\mathbf{x}, \mathbf{y}) : \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}, \mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}, \overline{\mathbf{y}}), \mathbf{y} \in \mathbb{Y}\right\},$$

is a convex optimization problem with respect to $\mathbf{y}$. $\quad\square$

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One great advantage of this property is that if $\mathbf{F}$, $\mathbf{f}$ and $\mathbf{g}$ are continuously differentiable and certain constraint qualification is satisfied, we can adopt KKT reformulation method, i.e., replacing this lower level problem by its KKT conditions. Hence, one more level reduction can be achieved, which ultimately leads to a single level equivalence of **R-PBL**. As such single optimization problem can readily be solved by a typical optimization package or a specialized solver for mathematical programs with equilibrium constraints, this computational scheme provides a remarkable convenience for practitioners. It is very different from a traditional understanding that those methods might not be able to solve **PBL**.

For **PBL** problems whose optimal solution may not exist, it has been proposed to compute their ϵ-approximations [23, 29] where $\mathbf{y} \in \mathbf{S}(\mathbf{x})$ in (3) is relaxed to

$$\mathbf{y} \in \mathbf{S}_\epsilon(\mathbf{x}) = \left\{ \mathbf{y} \in \mathbf{Y}(\mathbf{x}) : \mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \theta^*(\mathbf{x}) + \epsilon \right\}.$$

One benefit is that compared to the original **PBL** model, the ϵ-approximation could have an optimal solution, although not guaranteed. Another significant advantage is that the ϵ-approximation provides a modeling flexibility. It can be used to capture the upper level DM's safety margin consideration to hedge against deviations from the expected lower-level DM's decision [29]. Also, we note it can describe the lower level DM's tolerance level when he makes a non-cooperative decision against the upper level DM. When an optimal solution exists, the *Relaxation-and-Correction* can easily be employed to compute the ϵ-approximation with some minor modifications: (i) in (7), replace $\mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}, \overline{\mathbf{y}})$ by $\mathbf{f}(\mathbf{x}, \mathbf{y}) \leq \mathbf{f}(\mathbf{x}, \overline{\mathbf{y}}) + \epsilon$; ($ii$) in (9), replace $\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*) > \theta(\mathbf{x}^*)$ by $\mathbf{f}(\mathbf{x}^*, \overline{\mathbf{y}}^*) > \theta(\mathbf{x}^*) + \epsilon$; and ($iii$) in the optimization problem of the correction step, replace $\mathbf{f}(\mathbf{x}^*, \mathbf{y}) \leq \theta(\mathbf{x}^*)$ by $\mathbf{f}(\mathbf{x}^*, \mathbf{y}) \leq \theta(\mathbf{x}^*) + \epsilon$.

In the following, we apply our new computational scheme on the basic linear pessimistic problem and its variants. Because the correction step is rather standard and easy to implement, we mainly consider the relaxation step, i.e., their associated **R-PBL** formulations and computation.

3 Linear Pessimistic Bilevel Optimization Problems

In the remainder of this paper, we will focus on linear pessimistic problems where all constraints and objective functions are linear in $\mathbf{x}$ and $\mathbf{y}$. We first consider the basic linear **PBL** where the lower level problem is an LP and present its single level reformulation. We then extend our study to a few variants: linear mixed integer **PBL** where the lower level problem includes discrete variables, bilevel problem with coupled pessimistic constraints, and strong-weak bilevel problem.

3.1 Basic Linear PBL Problem

Consider the following linear pessimistic bilevel problem

$$\textbf{Linear} - \textbf{PBL}: \min \quad \mathbf{cx} + \max \ \mathbf{d}_1\mathbf{y} \tag{10}$$

$$\text{s.t.} \quad \mathbf{A}_1\mathbf{x} \le \mathbf{b}_1, \ \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d} \tag{11}$$

$$\mathbf{y} \in \mathbf{S}(\mathbf{x}) = \arg\min \left\{ \mathbf{d}_2\mathbf{y} : \mathbf{B}_2\mathbf{y} \le \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}, \ \mathbf{y} \in \mathbb{R}_+^m \right\} \tag{12}$$

where $n = n_c + n_d$, $\mathbf{A}_1, \mathbf{b}_1, \mathbf{A}_2, \mathbf{B}_2, \mathbf{b}_2, \mathbf{c}, \mathbf{d}_1$ and $\mathbf{d}_2$ are of appropriate dimensions. Let $\mathbf{X} = \{\mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d} : \mathbf{A}_1\mathbf{x} \le \mathbf{b}_1\}$ and

$$\Omega = \left\{ (\mathbf{x}, \mathbf{y}) \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d} \times \mathbb{R}_+^m : \mathbf{A}_1\mathbf{x} \le \mathbf{b}_1, \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\mathbf{y} \le \mathbf{b}_2 \right\}.$$

Unless explicitly stated, it is assumed in this paper that Ω is a non-empty compact set. Hence, for a given $\mathbf{x}$, set $\mathbf{Y}(\mathbf{x}) = \{\mathbf{y} \in \mathbb{R}_+^m : \mathbf{B}_2\mathbf{y} \le \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}\}$ is closed, if is not empty.

Remark: It is shown in [2] that if $\mathbf{x}$ are continuous, i.e., $n_d = 0$, the aforementioned assumption ensures the existence of an optimal solution. Indeed, through Branch-and-Bound method, this result can easily extends to a more general case where $\mathbf{x}$ are mixed integer variables, i.e., $n_d \ge 1$.

Next, because of the convexity of linear functions and Corollary 4, we can easily develop the following result using KKT reformulation. Note that superscript t is used to indicate matrix transpose operation, and $(\mathbf{u}, \pi)$ are dual variables introduced for KKT reformulation.

Corollary 5. *For* $\textbf{Linear} - \textbf{PBL}$ *problem, its tight* $\textbf{R-PBL}$ *relaxation is*

$$\min \quad \mathbf{cx} + \mathbf{d}_1\mathbf{y}$$

$$\textit{s.t.} \quad \mathbf{A}_1\mathbf{x} \le \mathbf{b}_1, \ \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\overline{\mathbf{y}} \le \mathbf{b}_2$$

$$\mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}} \in \mathbb{R}_+^m$$

$$\mathbf{y} \in \arg\max \left\{ \mathbf{d}_1\mathbf{y} : \mathbf{B}_2\mathbf{y} \le \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}, \ \mathbf{d}_2\mathbf{y} \le \mathbf{d}_2\overline{\mathbf{y}}, \ \mathbf{y} \in \mathbb{R}_+^m \right\}.$$

Let l be the dimension of $\mathbf{b}_2$. Then, this tight relaxation is equivalent to the following single level formulation

$$\min \quad \mathbf{cx} + \mathbf{d}_1\mathbf{y}$$

$$\textit{s.t.} \quad \mathbf{A}_1\mathbf{x} \le \mathbf{b}_1, \ \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\overline{\mathbf{y}} \le \mathbf{b}_2$$

$$\mathbf{A}_2\mathbf{x} + \mathbf{B}_2\mathbf{y} \le \mathbf{b}_2, \ \mathbf{d}_2\mathbf{y} - \mathbf{d}_2\overline{\mathbf{y}} \le 0, \ \mathbf{B}_2^t\mathbf{u} + \mathbf{d}_2^t\pi \ge \mathbf{d}_1^t$$

$$\mathbf{y} \perp (\mathbf{B}_2^t\mathbf{u} + \mathbf{d}_2^t\pi - \mathbf{d}_1^t), \ (\mathbf{u}, \pi) \perp (\mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_2\mathbf{y}, \mathbf{d}_2\overline{\mathbf{y}} - \mathbf{d}_2\mathbf{y})$$

$$\mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}} \in \mathbb{R}_+^m, \mathbf{y} \in \mathbb{R}_+^m, \mathbf{u} \in \mathbb{R}_+^l, \pi \in \mathbb{R}_+.$$

The last formulation is a mathematical program with linear complementarity constraints (MPCC). As previously mentioned, it can readily be solved by an optimization package specialized in this type of problems. Or, those linear complementarity constraints can be linearized using additional binary variables [4], which convert the whole formulation into a mixed integer

program (MIP) that can be easily handled by widely adopted professional MIP solver.

Sometimes, a bilevel problem involves multiple independent lower level DMs that have their own objective functions and constraints. It makes no difference to treat them as a single DM in the optimistic model as the resulting KKT reformulation still has a block structure where one block corresponds to one DM [11]. For **R-PBL** formulation, we do not suggest to aggregate them into a single DM to build a single lower level problem. Instead, we would rather treat them individually as

$$\mathbf{A}_2^i \mathbf{x} + \mathbf{B}_2^i \overline{\mathbf{y}}^i \leq \mathbf{b}_2^i, \text{ and, } \mathbf{y}^i \in \arg\max \left\{ \mathbf{d}_1^i \mathbf{y}^i : \mathbf{B}_2^i \mathbf{y}^i \leq \mathbf{b}_2^i - \mathbf{A}_2^i \mathbf{x}, \mathbf{d}_2^i \mathbf{y}^i \leq \mathbf{d}_2^i \overline{\mathbf{y}}^i, \mathbf{y}^i \in \mathbb{R}_+^m \right\},$$

where superscript i is used to indicate the ith lower level DM's parameters and variables. Note that KKT reformulation can be applied to individual lower level problems, which preserves the block structure that is friendly to decomposition algorithms.

3.2   Mixed Integer PBL Problem

Consider the general mixed integer **PBL** where the lower level problem has discrete variables. Let $\mathbf{y} = (\mathbf{y}_c, \mathbf{y}_d)$ where $\mathbf{y}_c$ and $\mathbf{y}_d$ are continuous and discrete variables of $\mathbf{y}$ with m_c and m_d being their dimensions respectively. Then, we represent the corresponding expressions in (10) and (12) as

$$\min \mathbf{cx} + \max(\mathbf{d}_{1c} \mathbf{y}_c + \mathbf{d}_{1d} \mathbf{y}_d),$$

and

$$\mathbf{S}(\mathbf{x}) = \arg\min \left\{ \mathbf{d}_{2c} \mathbf{y}_c + \mathbf{d}_{2d} \mathbf{y}_d : \mathbf{B}_{2c} \mathbf{y}_c + \mathbf{B}_{2d} \mathbf{y}_d \leq \mathbf{b}_2 - \mathbf{A}_2 \mathbf{x}, \ \mathbf{y}_c \in \mathbb{R}_+^{m_c}, \mathbf{y}_d \in \mathbb{Z}_+^{m_d} \right\}. \quad (13)$$

We also denote the whole formulation as **MIP − PBL**.

As mentioned in Section 2.1 that the construction of **R-PBL** relaxation does not rely on the convexity of the lower level problem, we next provides that tight relaxation of **MIP − PBL**.

Corollary 6. *For* **MIP − PBL** *problem, its tight* **R-PBL** *relaxation is*

$$\min \quad \mathbf{cx} + \mathbf{d}_{1c} \mathbf{y}_c + \mathbf{d}_{1d} \mathbf{y}_d \tag{14}$$

$$s.t. \quad \mathbf{A}_1 \mathbf{x} \leq \mathbf{b}_1, \ \mathbf{A}_2 \mathbf{x} + \mathbf{B}_{2c} \overline{\mathbf{y}}_c + \mathbf{B}_{2d} \overline{\mathbf{y}}_d \leq \mathbf{b}_2 \tag{15}$$

$$\mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}}_c \in \mathbb{R}_+^{m_c}, \overline{\mathbf{y}}_d \in \mathbb{Z}_+^{m_d} \tag{16}$$

$$(\mathbf{y}_c, \mathbf{y}_d) \in \arg\max \left\{ \mathbf{d}_{1c} \mathbf{y}_c + \mathbf{d}_{1d} \mathbf{y}_d : \right. \tag{17}$$

$$\mathbf{B}_{2c} \overline{\mathbf{y}}_c + \mathbf{B}_{2d} \overline{\mathbf{y}}_d \leq \mathbf{b}_2 - \mathbf{A}_2 \mathbf{x}, \quad \mathbf{d}_{2c} \mathbf{y}_c + \mathbf{d}_{2d} \mathbf{y}_d \leq \mathbf{d}_{2c} \overline{\mathbf{y}}_c + \mathbf{d}_{2d} \overline{\mathbf{y}}_d \tag{18}$$

$$\left. \mathbf{y}_c \in \mathbb{R}_+^{m_c}, \mathbf{y}_d \in \mathbb{Z}_+^{m_d} \right\}. \tag{19}$$

In the aforementioned bilevel MIP formulation, because of the existence of discrete variables in the lower level problem, it is not feasible to apply the popular KKT reformulation method to derive a single level equivalent model. Indeed, even for the less complicated optimistic bilevel MIP, it may not have any optimal solution [22]. We discuss next making a few modifications

on this formulation so that we can employ a recent solution procedure to compute exact or strong approximate solution [30].

By taking advantage of the minimax structure in the objective function (14) with respect to (17), we equivalently modify it as $\min \mathbf{cx} + \eta$, and convert the set membership restriction in (17) into the following inequality

$$\eta \geq \max \left\{ \mathbf{d}_{1c}\mathbf{y}_c + \mathbf{d}_{1d}\mathbf{y}_d : (18-19) \right\}. \tag{20}$$

We mention that although they are trivial modifications, the resulting new representation eliminates the necessity to duplicate lower level variables for simulation in the standard solution procedure [30].

A sufficient condition ensuring the existence of an optimal solution is that the lower level problem has the *relatively complete response* property. In our context, this property is that for any possible $(\mathbf{x}, \overline{\mathbf{y}}_{\mathbf{c}}, \overline{\mathbf{y}}_{\mathbf{d}}, \mathbf{y}_{\mathbf{d}})$, the remaining lower level problem defined in (17-19), which is its LP portion, has an finite optimal value. Actually, in our case such property does not hold in general. Note that for a fixed $\mathbf{x}^*$, if $(\overline{\mathbf{y}}_c^*, \overline{\mathbf{y}}_d^*)$ is an optimal solution of the original lower level problem in the $\mathbf{MIP-PBL}$ model, it is the most case that the second constraint in (18) will cause the LP lower level problem infeasible when $\mathbf{y}_d \neq \overline{\mathbf{y}}_d^*$. Hence, we have to introduce *artificial variables*, which are to be penalized with big-M coefficients, that allow constraint violations in (18). Specifically, we further modify the bilevel restriction in (20) as the following, where $\mathbf{1}$ is the l-dimensional all-ones row vector and $\mathbf{I}$ is the $l \times l$ identity matrix.

$$\eta \geq \max \left\{ \mathbf{d}_{1c}\mathbf{y}_c + \mathbf{d}_{1d}\mathbf{y}_d - M\mathbf{1}\mathbf{y}_a - My_f : \right. \tag{21}$$

$$\mathbf{B}_{2c}\mathbf{y}_c + \mathbf{B}_{2d}\mathbf{y}_d - \mathbf{I}\mathbf{y}_a \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}, \quad \mathbf{d}_{2c}\mathbf{y}_c + \mathbf{d}_{2d}\mathbf{y}_d - y_f \leq \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d \tag{22}$$

$$\mathbf{y}_a \in \mathbf{R}_+^l, \ \mathbf{y}_c \in \mathbb{R}_+^{m_c}, \ \mathbf{y}_d \in \mathbb{Z}_+^{m_d}, y_f \in \mathbf{R}_+ \left. \right\}. \tag{23}$$

As a result, the *extended reformulation* of the bilevel MIP model in Corollary 6 is

$$\min \left\{ \mathbf{cx} + \eta : (15-16), \ (21-23) \right\}, \tag{24}$$

which can then be solved by the reformulation and decomposition method in [30], a procedure that is easily implementable with an optimization package for MPCC or an MIP solver.

Remark: It has been shown in [30] that if the bilevel MIP model has an optimal solution, it can be found by setting M to a large value in (24). Otherwise, an ϵ-optimal solution can be derived by adjusting the value of M. One example of the latter case can be found in Section 4. To keep the paper self-contained, we provide the tailored procedure for (24) in the appendix.

3.3 Bilevel Problem with Coupled Pessimistic Constraints

One type bilevel problem with coupled constraints studied in [27, 29], under the linear settings, is formulated as

$$\mathbf{CP} : \min \ \mathbf{cx} \tag{25}$$

$$\text{s.t. } \mathbf{A}_1 \mathbf{x} \leq \mathbf{b}_1, \ \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d} \tag{26}$$

$$\mathbf{f}^i \mathbf{x} + \mathbf{g}^i \mathbf{y} \leq t^i, \ \forall \mathbf{y} \in \arg\min_{\mathbf{y}} \left\{ \mathbf{d}^i \mathbf{y} : \mathbf{Q}^i \mathbf{y} \leq \mathbf{h}^i - \mathbf{P}^i \mathbf{x}, \mathbf{y} \geq 0 \right\}, \ i = 1, \ldots, p \tag{27}$$

where $\mathbf{f}^i$ and $\mathbf{g}^i$ are row vectors (like $\mathbf{c}$ in the objective function (25)) for all i. The optimization problem defining $\mathbf{y}$ in (27) is called as the ith lower level problem. Different from the conventional concept in optimistic models that the coupled constraints over $\mathbf{x}$ and $\mathbf{y}$, which appear in the upper level problem, should just be satisfied by *the* selected optimal $\mathbf{y}$, constraints in (27) are rather pessimistic as they must be satisfied by *all* optimal $\mathbf{y}$ of the associated lower level problems. In this regard, $\mathbf{CP}$'s solution is just in $\mathbf{x}$ space, not in $(\mathbf{x}, \mathbf{y})$ space.

As mentioned, it is argued in [27, 29] that this type of formulation generalizes the standard **PBL** in (1-3). Also, for a special independent case where $\mathbf{P}^i$s are missing in those constraints, an iterative solution procedure using semi-infinite programming tools is developed [27, 29]. Next, by using the technique developed in Section 2, we show that the general dependent $\mathbf{CP}$ model can be reformulated into a format that is directly computable for many off-the-shelf packages or solvers.

Assume that $\mathbf{Y}^i(\mathbf{x}) = \{\mathbf{y} \in \mathbf{R}_+^{m_i} : \mathbf{Q}^i \mathbf{y} \leq \mathbf{h}^i - \mathbf{P}^i \mathbf{x}\}$ is a non-empty compact set for $\mathbf{x} \in \mathbf{X}$. Instead of using "$\forall$" operation to describe the ith coupled constraint in (27), we can represent it through pessimistic bilevel optimization as the following:

$$\mathbf{f}^i \mathbf{x} + \max_{\mathbf{y} \in \mathbf{S}^i(\mathbf{x})} \mathbf{g}^i \mathbf{y} \leq t^i,$$

where $\mathbf{S}^i(\mathbf{x}) = \arg\min\{\mathbf{d}^i \mathbf{y} : \mathbf{Q}^i \mathbf{y} \leq \mathbf{h}^i - \mathbf{P}^i \mathbf{x}, \ \mathbf{y} \geq 0\}$. As a result, using arguments similar to those presented in Section 2.1, the next result can be easily proven.

Lemma 7. *For a fixed* $\mathbf{x}^* \in \mathbf{X}$*, it satisfies the* i^{th} *constraint in* (27) *if and only if there exist* $\overline{\mathbf{y}}^{i*} \in \mathbb{R}_+^{m_i}$ *and* $\mathbf{y}^{i*} \in \arg\max\{\mathbf{g}^i \mathbf{y} : \mathbf{Q}^i \mathbf{y} \leq \mathbf{h}^i - \mathbf{P}^i \mathbf{x}^*, \ \mathbf{d}^i \mathbf{y} \leq \mathbf{d}^i \overline{\mathbf{y}}^{i*}, \mathbf{y} \in \mathbf{R}_+^{m_i}\}$*, and they satisfy the following constraints*

$$\mathbf{Q}^i \overline{\mathbf{y}}^{i*} \ \leq \ \mathbf{h}^i - \mathbf{P}^i \mathbf{x}^*, \tag{28}$$

$$\mathbf{g}^i \mathbf{y}^{i*} \ \leq \ t^i - \mathbf{f}^i \mathbf{x}^*. \tag{29}$$

We mention that superscript i is used in $\overline{\mathbf{y}}^i$ and $\mathbf{y}^i$ to indicate that those variables and associated constraints are introduced specifically for the ith coupled constraint. So, if multiple coupled constraints exist, this equivalence result should be applied constraint-wise. Based on Lemma 7 and using KKT reformulation, we can convert the $\mathbf{CP}$ model into a computationally friendly formulation.

Corollary 8. *Let* l_i *be the dimension of* $\mathbf{h}^i$*. The* $\mathbf{CP}$ *model defined in (25-27) is equivalent*

to the following single-level formulation.

$$\min \ \mathbf{c}\mathbf{x}$$

$$s.t. \ \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}$$

$$\mathbf{P}^i\mathbf{x} + \mathbf{Q}^i\overline{\mathbf{y}}^i \leq \mathbf{h}^i, \ \mathbf{f}^i\mathbf{x} + \mathbf{g}^i\mathbf{y}^i \leq t^i, \ i = 1, \ldots, p$$

$$\mathbf{P}^i\mathbf{x} + \mathbf{Q}^i\mathbf{y}^i \leq \mathbf{h}^i, \ \mathbf{d}^i\mathbf{y}^i - \mathbf{d}^i\overline{\mathbf{y}}^i \leq 0, \ (\mathbf{P}^i)^t\mathbf{u}^i + (\mathbf{d}^i)^t\pi^i \geq (\mathbf{g}^i)^t, \ i = 1, \ldots, p$$

$$\mathbf{y}^i \perp \left((\mathbf{P}^i)^t\mathbf{u}^i + (\mathbf{d}^i)^t\pi^i - (\mathbf{g}^i)^t \right), \ i = 1, \ldots, p$$

$$(\mathbf{u}^i, \pi^i) \perp \left(\mathbf{h}^i - \mathbf{P}^i\mathbf{x} - \mathbf{Q}^i\mathbf{y}^i, \mathbf{d}^i\overline{\mathbf{y}}^i - \mathbf{d}^i\mathbf{y}^i \right), \ i = 1, \ldots, p$$

$$\overline{\mathbf{y}}^i \in \mathbb{R}_+^{m_i}, \mathbf{y}^i \in \mathbb{R}_+^{m_i}, \mathbf{u}^i \in \mathbb{R}_+^{l_i}, \pi^i \in \mathbb{R}_+, \ i = 1, \ldots, p.$$

Remark: (i) The reason we say that the aforementioned formulation is equivalent to **CP** is that the $\mathbf{x}$ portion of its optimal solution and its optimal value are optimal to **CP**. (ii) Note that we can deal with the nonlinear complementarity constraints in the aforementioned formulation by Branch-and-Bound or by enumerating the implied linear constraints, both of which are finite. Hence, it can be inferred that this formulation, as well as **CP**, either has an optimal solution, or is infeasible. Again, it can be directly computed by an MPCC optimization package or by any professional MIP solver, after linearization. (iii) If the non-empty assumption on $\mathbf{Y}^i(\mathbf{x})$ for $\mathbf{x} \in \mathbb{X}$ is not satisfied, similar to the modifications made in (21- 23), we can include artificial variables with big-M coefficients so that (29) is of a very negative left-hand-side value (through the help of artificial variables) whenever $\mathbf{x}$ causes set $\mathbf{Y}^i(\mathbf{x})$ empty.

3.4 Strong-Weak Bilevel Problem

Noting that the solution to the lower level problem might not be unique, the strong-weak bilevel optimization problem, also known as partially cooperative bilevel model, has been proposed and investigated in [1, 12, 31]. It integrates the optimistic and pessimistic formulations through a weighted summation, where the weight coefficient can be interpreted as the cooperative probability of the lower level DM. Hence, knowing that the lower level DM just cooperates partially or stochastically, the upper level DM, instead of being completely optimistic or pessimistic, solves the strong-weak bilevel problem to derive an intermediate solution. Actually, it is interesting to observe that there exist situations where the lower level DM achieves his best interest by being partially or stochastically cooperative [12]. We believe that the strong-weak model has its significance in modeling and analyzing real situations.

Let β represent the weight parameter. The formulation of the strong-weak bilevel optimization problem is

$$\mathbf{SW} - \mathbf{PBL}: \ \min \quad \mathbf{c}\mathbf{x} + \beta f_1 + (1 - \beta)f_2$$

$$\text{s.t.} \quad \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}$$

$$f_1 = \min \left\{ \mathbf{d}_1\mathbf{y} : \mathbf{y} \in \mathbf{S}(\mathbf{x}) \right\}, \ f_2 = \max \left\{ \mathbf{d}_1\mathbf{y} : \mathbf{y} \in \mathbf{S}(\mathbf{x}) \right\}$$

where $\mathbf{S}(\mathbf{x})$ is defined as in (12).

Remark: It is shown in [12, 31] that $\mathbf{SW} - \mathbf{PBL}$ has an optimal solution if $\mathbf{x}$ are continuous, i.e., $n_d = 0$. Again, through Branch-and-Bound argument, this result extends to a more general case where $\mathbf{x}$ are mixed integer variables. Also, we would rather say its solution is simply in $\mathbf{x}$ space as the lower level DM's decision is not certain in general.

To solve $\mathbf{SW} - \mathbf{PBL}$ problem, a couple of penalty methods have been developed in [12, 31], which iteratively adjust penalty coefficients and compute the resulting relaxations to ensure the convergence to an optimal solution. Again, using arguments from Section 2.1 and KKT reformulation, we provide its tight $\mathbf{R\text{-}PBL}$ relaxation and the computationally friendly single level reformulation. Variable $\mathbf{y}^o$ and $\mathbf{y}^p$ are introduced to represent those in optimistic and pessimistic parts, respectively.

Corollary 9. *For* $\mathbf{SW} - \mathbf{PBL}$ *problem, its* $\mathbf{R\text{-}PBL}$ *model is*

$$
\begin{aligned}
\min \quad & \mathbf{cx} + \beta f_1 + (1 - \beta)f_2 \\
s.t. \quad & \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d} \\
& \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\overline{\mathbf{y}} \leq \mathbf{b}_2, \overline{\mathbf{y}} \in \mathbb{R}_+^m \\
& f_1 \geq \mathbf{d}_1\mathbf{y}^o, \ \mathbf{y}^o \in \mathbf{S}(\mathbf{x}) \\
& f_2 \geq \mathbf{d}_1\mathbf{y}^p, \ \mathbf{y}^p \in \max\left\{ \mathbf{d}_1\mathbf{y}^p : \mathbf{B}_2\mathbf{y}^p \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}, \ \mathbf{d}_2\mathbf{y}^p \leq \mathbf{d}_2\overline{\mathbf{y}}, \ \mathbf{y}^p \in \mathbb{R}_+^m \right\},
\end{aligned}
$$

which is equivalent to the following single level formulation

$$
\begin{aligned}
\min \quad & \mathbf{cx} + \beta f_1 + (1 - \beta)f_2 \\
s.t. \quad & \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\overline{\mathbf{y}} \leq \mathbf{b}_2, \ f_1 \geq \mathbf{d}_1\mathbf{y}^o, \ f_2 \geq \mathbf{d}_1\mathbf{y}^p \\
& \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\mathbf{y}^o \leq \mathbf{b}_2, \ \mathbf{B}_2^t\mathbf{v} \leq \mathbf{d}_2^t, \ \mathbf{y}^o \perp (\mathbf{d}_2^t - \mathbf{B}_2^t\mathbf{v}), \ \mathbf{v} \perp (\mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_2\mathbf{y}^o) \\
& \mathbf{A}_2\mathbf{x} + \mathbf{B}_2\mathbf{y}^p \leq \mathbf{b}_2, \ \mathbf{d}_2\mathbf{y}^p \leq \mathbf{d}_2\overline{\mathbf{y}}, \ \mathbf{B}_2^t\mathbf{u} + \mathbf{d}_2^t\pi \geq \mathbf{d}_1^t \\
& \mathbf{y}^p \perp (\mathbf{B}_2^t\mathbf{u} + \mathbf{d}_2^t\pi - \mathbf{d}_1^t), \ (\mathbf{u}, \pi) \perp (\mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_2\mathbf{y}^p, \mathbf{d}_2\overline{\mathbf{y}} - \mathbf{d}_2\mathbf{y}^p) \\
& \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}} \in \mathbb{R}_+^m, \mathbf{y}^o \in \mathbb{R}_+^m, \mathbf{y}^p \in \mathbb{R}_+^m, (-\mathbf{v}) \in \mathbf{R}_+^l, \mathbf{u} \in \mathbb{R}_+^l, \pi \in \mathbb{R}_+. \qquad \square
\end{aligned}
$$

Remark: (i) Again, the aforementioned single level formulation can be directly computed by an MPCC optimization package or by an MIP solver. (ii) An equivalent single level formulation can also be obtained if we explicitly impose the optimality requirement with respect to $\mathbf{d}_2\overline{\mathbf{y}}$ on $\overline{\mathbf{y}}$, and set $f_1 \geq \mathbf{d}_1\overline{\mathbf{y}}$, which allows us to eliminate variables $\mathbf{y}^o$ and related constraints. The reason that we prefer the one in Corollary 9 is that the optimistic and pessimistic parts can be computed independently for a given $\mathbf{x}$. Indeed, for the situation where the optimality requirement is not directly available, e.g., a strong-weak formulation with an MIP lower level problem, we still can make use of the primal information of the lower level problem represented by $\overline{\mathbf{y}}$ and associated constraints to effective compute the pessimistic portion, which is independent of the solution quality of $\mathbf{y}^o$.

4 Numerical Study

In this section, we make use of the developed computing scheme to solve instances of linear **PBL** and its variants. Given that the core computation reduces to solving a regular (optimistic) bilevel optimization problem, which has a large number of algorithms and methods, our numerical study just serves the demonstration purpose of this scheme, rather than to provide a comprehensive investigation. For all instances, CPLEX Mixed Integer Program Solver 12.5 is adopted as our computational platform, which is used to solve their (linearized) KKT conditions based reformulations.

Example 1. *Consider the following pessimistic linear bilevel problem adopted from [12].*

$$\min \quad -8x_1 - 6x_2 + \max(-25y_1 - 30y_2 + 2y_3 + 16y_4) \tag{30}$$

$$s.t. \quad x_1 + x_2 \le 10, \ x_1, x_2 \ge 0 \tag{31}$$

$$(y_1, y_2, y_3, y_4) \in \mathbf{S}(x_1, x_2) = \arg\min\Big\{ -10y_1 - 10y_2 - 10y_3 - 10y_4 : \tag{32}$$

$$y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2, \ -y_1 + y_4 \le 0.8x_1 + 0.8x_2 \tag{33}$$

$$y_2 + y_4 \le 4x_2, \ y_1, y_2, y_3, y_4 \ge 0 \Big\}. \tag{34}$$

*According to Corollary 5, the associated **R-PBL** model is*

$$\min -8x_1 - 6x_2 - 25y_1 - 30y_2 + 2y_3 + 16y_4$$

$$s.t. \ x_1 + x_2 \le 10, \ \overline{y}_1 + \overline{y}_2 + \overline{y}_3 + \overline{y}_4 \le 10 - x_1 - x_2, \ -\overline{y}_1 + \overline{y}_4 \le 0.8x_1 + 0.8x_2, \ \overline{y}_2 + \overline{y}_4 \le 4x_2$$

$$x_1, x_2 \ge 0, \ \overline{y}_1, \overline{y}_2, \overline{y}_3, \overline{y}_4 \ge 0$$

$$(y_1, y_2, y_3, y_4) \in \arg\max\Big\{ -25y_1 - 30y_2 + 2y_3 + 16y_4 : \ y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2,$$

$$-y_1 + y_4 \le 0.8x_1 + 0.8x_2, \ y_2 + y_4 \le 4x_2,$$

$$-10y_1 - 10y_2 - 10y_3 - 10y_4 \le -10\overline{y}_1 - 10\overline{y}_2 - 10\overline{y}_3 - 10\overline{y}_4, \ y_1, y_2, y_3, y_4 \ge 0 \Big\}$$

By solving its single level KKT reformulation (through linearizing the complementarity constraints and computing the resulting MIP problem) in the form of that in Corollary 5, we obtain an optimal solution with $x_1^* = 10, x_2^* = 0, \overline{y}_j^* = y_j^* = 0$ for $j = 1, \dots, 4$, and the optimal value equal to -80. Because we have

$$-10\overline{y}_1^* - 10\overline{y}_2^* - 10\overline{y}_3^* - 10\overline{y}_4^* = 0$$

$$= \min\Big\{ -10y_1 - 10y_2 - 10y_3 - 10y_4 :$$

$$y_1 + y_2 + y_3 + y_4 \le 0, \ -y_1 + y_4 \le 8, y_2 + y_4 \le 0, \ y_1, y_2, y_3, y_4 \ge 0 \Big\},$$

we can conclude that the $\mathbf{y}^*$-portion is optimal to the lower level problem and the correction step can simply be ignored. Finally, we report $(x_1, x_2, y_1, y_2, y_3, y_4) = (10, 0, 0, 0, 0, 0)$ as an optimal solution to the original pessimistic problem.

As demonstrated next, it is not always the case that we can neglect the correction step.

Example 2. *Consider a modification of (30-34) where the objective function in (30) is changed*

to min $0x_1 + 0x_2 + \max(-2y_1 - 3y_2 - 2y_3 - 16y_4)$. *By repeating the same solution procedure, we obtain an optimal solution with $x_1^* = x_2^* = 0$ and $\overline{y}_j^* = 0$ for $j = 1, \ldots, 4$, and $y_1^* = 10, y_j^* = 0$ for j=2,3,4. Note that*

$$- 10\overline{y}_1^* - 10\overline{y}_2^* - 10\overline{y}_3^* - 10\overline{y}_4^* = 0$$

$$> -100 = \min\Big\{ - 10y_1 - 10y_2 - 10y_3 - 10y_4 :$$

$$y_1 + y_2 + y_3 + y_4 \le 10, \ -y_1 + y_4 \le 0, y_2 + y_4 \le 0, \ y_1, y_2, y_3, y_4 \ge 0\Big\},$$

which suggests that $(y_1^*, y_2^*, y_3^*, y_4^*)$ might not be optimal to the lower level problem. Hence, according to (9), we perform the correction step and derive an optimal solution (which is identical to $(x_1, x_2, y_1, y_2, y_3, y_4) = (0, 0, 10, 0, 0, 0)$) for this pessimistic bilevel problem. Certainly, as discussed after the relaxation-and-correction scheme, we can compare the value of $-10y_1^* - 10y_2^* - 10y_3^* - 10y_4^*$ and the optimal value of the lower level problem, which allows us to ignore the correction step for this instance.

In the following, we solve a mixed integer **PBL** instance.

Example 3. *Consider the next instance that is extended from (30-34) with a new constraint on (x_1, x_2) in the upper level and an integer variable restriction on y_3 in the lower level. So, the lower level problem is a mixed integer program.*

$$\begin{aligned}
\min \quad & -8x_1 - 6x_2 + \max(-25y_1 - 30y_2 + 2y_3 + 16y_4) \\
\text{s.t.} \quad & x_1 + x_2 \le 10, \ 2x_1 + 5x_2 \le 13, \ x_1, x_2 \ge 0 \\
& (y_1, y_2, y_3, y_4) \in \mathbf{S}(x_1, x_2) = \arg\min\Big\{ - 10y_1 - 10y_2 - 10y_3 - 10y_4 : \\
& y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2, \ -y_1 + y_4 \le 0.8x_1 + 0.8x_2 \\
& y_2 + y_4 \le 4x_2, \ y_1, y_2, y_4 \ge 0, \ y_3 \in \mathbb{Z}_+\Big\}.
\end{aligned}$$

*The extended formulation of its tight **R-PBL** relaxation with artificial variables is*

$$\begin{aligned}
\min \quad & -8x_1 - 6x_2 + \eta \\
\text{s.t.} \quad & x_1 + x_2 \le 10, \ 2x_1 + 5x_2 \le 13, \ x_1 + x_2 + \overline{y}_1 + \overline{y}_2 + \overline{y}_3 + \overline{y}_4 \le 10 \\
& -0.8x_1 - 0.8x_2 - \overline{y}_1 + \overline{y}_4 \le 0, \ -4x_2 + \overline{y}_2 + \overline{y}_4 \le 0 \\
& x_1, x_2 \ge 0, \ \overline{y}_1, \overline{y}_2, \overline{y}_4 \ge 0, \ \overline{y}_3 \in \mathbb{Z}_+ \\
& \eta \ge \max\Big\{ - 25y_1 - 30y_2 + 2y_3 + 16y_4 - My_{a1} - My_{a2} - My_{a3} - My_f : \\
& y_1 + y_2 + y_3 + y_4 - y_{a1} \le 10 - x_1 - x_2, \ -y_1 + y_4 - y_{a2} \le 0.8x_1 + 0.8x_2 \\
& y_2 + y_4 - y_{a3} \le 4x_2, \ -10y_1 - 10y_2 - 10y_3 - 10y_4 - y_f \le -10\overline{y}_1 - 10\overline{y}_2 - 10\overline{y}_3 - 10\overline{y}_4 \\
& y_1, y_2, y_4, y_{a1}, y_{a2}, y_{a3}, y_f \ge 0, \ y_3 \in \mathbb{Z}_+\Big\},
\end{aligned}$$

where M is set to $5,000$ in our numerical study. Using the procedure described in the appendix to compute the aforementioned bilevel mixed integer program, we obtain an optimal solution with $x_1^* = 6.005$, $x_2^* = 0$, $\overline{y}_1^* = 3.995$, $\overline{y}_2^* = \overline{y}_3^* = \overline{y}_4^* = 0$, $y_1^* = 0.995$, $y_2^* = y_4^* = 0$ and $y_3^* = 3$, and the corresponding optimal value is -66.915. Then, deriving the optimal value of

the original lower level problem given (x_1^*, x_2^*) and comparing it with respect to $-10\overline{y}_1^* - 10\overline{y}_2^* - 10\overline{y}_3^* - 10\overline{y}_4^*$, it can be seen that the correction step is not needed.

The close proximity of x_1^* to an integer value indicates that the solution is ϵ-optimal and this **PBL** instance does not have any exact solution. In the following, we provide an analysis to confirm that it is the actual situation. First, we consider the original lower level problem for any feasible (x_1, x_2). Because of the connection between the objective function and the first constraint, it is easy to see that an optimal solution can always be obtained by setting $y_1 = 10 - x_1 - x_2$ and the associated optimal value is $-10(10 - x_1 - x_2)$. Hence, the original three level **PBL** can be simplified as a regular bilevel problem

$$
\begin{aligned}
\min \quad & -8x_1 - 6x_2 + \eta \\
\text{s.t.} \quad & x_1 + x_2 \leq 10, \ 2x_1 + 5x_2 \leq 13, \ x_1, x_2 \geq 0 \\
& \eta \geq \max\Big\{ -25y_1 - 30y_2 + 2y_3 + 16y_4 : \ y_1 + y_2 + y_3 + y_4 = 10 - x_1 - x_2 \\
& -y_1 + y_4 \leq 0.8x_1 + 0.8x_2, \ y_2 + y_4 \leq 4x_2, \ y_1, y_2, y_4 \geq 0, \ y_3 \in \mathbb{Z}_+ \Big\}.
\end{aligned}
$$

Moreover, comparing y_1 and y_2's roles in the objective function and constraints, it follows that $y_2 = 0$ in any optimal solution and the constraint with the lower level problem can be further modified to

$$
\begin{aligned}
\eta \geq \max\Big\{ & -25y_1 + 2y_3 + 16y_4 : \ y_1 + y_3 + y_4 = 10 - x_1 - x_2 \\
& -y_1 + y_4 \leq 0.8x_1 + 0.8x_2, \ y_4 \leq 4x_2, \ y_1, y_4 \geq 0, \ y_3 \in \mathbb{Z}_+ \Big\} \\
= \max\Big\{ & 2y_3 + \omega : \\
& y_3 \leq 10 - x_1 - x_2, \ y_3 \in \mathbb{Z}_+ \\
& \omega = \max\{ -25y_1 + 16y_4 : \ y_1 + y_4 = 10 - x_1 - x_2 - y_3, \ -y_1 + y_4 \leq 0.8x_1 + 0.8x_2 \\
& y_4 \leq 4x_2, \ y_1, y_4 \geq 0 \} \Big\}
\end{aligned}
$$

We separate y_3 from other variables as its possible values can be enumerated. In case that $y_3 \leq 10 - x_1 - x_2$ is violated for a particular y_3', we can set its corresponding value to $-\infty$ by convention. Otherwise, the linear program problem defining ω is feasible. The feasible set and the optimal solution is displayed in Figure 1, where two critical points A and B are intersections of the first and second constraints, and the first and third constraints, respectively. Their analytical expressions are

$$(y_1, y_4)_A = (5 - 0.9x_1 - 0.9x_2 - 0.5y_3, 5 - 0.1x_1 - 0.1x_2 - 0.5y_3), \ (y_1, y_4)_B = (10 - x_1 - 5x_2 - y_3, 4x_2).$$

The one with the smaller y_4 coordinate, along with the line segment $Q - P$, defines the feasible set, which is the bold line in Figure 1. Noting that the dot line represents an iso-profit line and the arrow represents the increasing direction to maximize ω, it is clear that either point A or B will be the optimal solution, which leads to

$$\omega = -45 + 20.9x_1 + 20.9x_2 + 4.5y_3, \ \text{or} \ \omega = -250 + 25x_1 + 189x_2 + 25y_3.$$

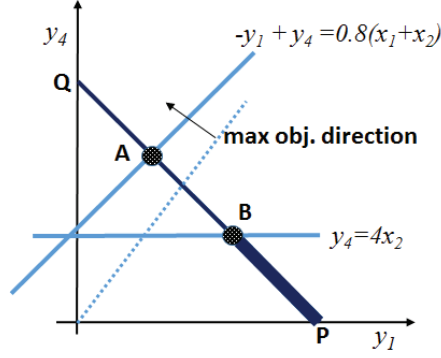In either case, we can, without changing y_3's feasibility (or infeasibility) status, always decrease

Figure 1: Solution of (y_1, y_4)

x_2 and add the decreased quantity to x_1 to achieve the same or a better (i.e., smaller) value for ω. So, it is sufficient to fix $x_2 = 0$ for the upper level, which actually renders point B as the optimal solution and $\omega = -250 + 25x_1 + 25y_3$. As a result the original **PBL** reduces to the following problem

$$
\begin{aligned}
\min \quad & -8x_1 + \eta \\
\text{s.t.} \quad & x_1 \leq 10, \ 2x_1 \leq 13, \ x_1 \geq 0 \\
& \eta \geq \begin{cases} 27y_3 - 250 + 25x_1, & \text{if } x_1 + y_3 \leq 10 \\ -\infty, & \text{otherwise} \end{cases} \\
& \text{for } y_3 = 0, \ldots, 10.
\end{aligned}
$$

With this formulation, the interaction between x_1 and y_3 and the resulting objective function value can be easily analyzed. Let $x = k + \epsilon$ with $k \in 0, \ldots, 6$ and $0 < \epsilon \leq 1$ ($\epsilon \leq 0.5$ if $k = 6$). Then, feasible values for y_3 are $0, \ldots, 10 - k - 1$ and the associated objective function value is $-250 + 17x_1 + 27 \max\{0, \ldots, 10 - k - 1\} = -7 + 17x_1 - 27k = -10k - 7 + 17\epsilon$. Clearly, the best possible objective function value is achieved when $k = 6$. Moreover, the smaller ϵ, the better (i.e., less) objective function value, which causes the infimum to be -67. However, this infimum cannot be achieved. When $\epsilon > 0$, feasible values for y_3 are $\{0, 1, 2, 3\}$, while when $\epsilon = 0$, feasible values for y_3 becomes $\{0, 1, 2, 3, 4\}$. For the latter case, the objective function value equals $-250 + 17 * 6 + 27 \max\{0, 1, 2, 3, 4\} = -40$. Hence, with the aforementioned analysis, it can be confirmed that this **PBL** instance does not have any exact solution.

Note that when $\epsilon = 0.005$, the associated ϵ-optimal value is -66.915, which matches the pessimistic result computed in Example 3. Interestingly, the optimistic counterpart of this instance actually has an optimal solution with $x_1 = 0$, $x_2 = 2$, $y_1 = y3 = y_4 = 0$ and $y_3 = 8$, and the corresponding optimal value is -252.

Next, we consider an instance of bilevel problem with a coupled pessimistic constraint.

Example 4. *Consider the following problem*

$$\min \quad -8x_1 - 6x_2$$

$$\text{s.t.} \quad x_1 + x_2 \le 10, \ x_1, x_2 \ge 0$$

$$2x_1 + x_2 - y_1 - y_2 - y_3 - y_4 \le 0, \ \forall (y_1, y_2, y_3, y_4) \in \mathbf{S}(x_1, x_2)$$

where $\mathbf{S}(x_1, x_2)$ *in the coupled constraint is defined as in (32-34). Note that* $\mathbf{Y}(x_1, x_2) = \{(y_1, y_2, y_3, y_4) \in \mathbb{R}_+^4 : y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2, \ -y_1 + y_4 \le 0.8x_1 + 0.8x_2, \ y_2 + y_4 \le 4x_2\}$ *is a non-empty compact set for any feasible* (x_1, x_2). *Then, according to Lemma 7, we can reformulate the whole bilevel problem as*

$$\min \quad -8x_1 - 6x_2$$

$$\text{s.t.} \quad x_1 + x_2 \le 10, \ \overline{y}_1 + \overline{y}_2 + \overline{y}_3 + \overline{y}_4 + x_1 + x_2 \le 10$$

$$-\overline{y}_1 + \overline{y}_4 - 0.8x_1 - 0.8x_2 \le 0, \ \overline{y}_2 + \overline{y}_4 - 4x_2 \le 0$$

$$2x_1 + x_2 + \max_{(y_1, y_2, y_3, y_4) \in \tilde{\mathbf{Y}}(x_1, x_2, \overline{y}_1, \overline{y}_2, \overline{y}_3, \overline{y}_4)} (-y_1 - y_2 - y_3 - y_4) \le 0$$

$$x_1, x_2, \overline{y}_1, \overline{y}_2, \overline{y}_3, \overline{y}_4 \ge 0$$

where $\tilde{\mathbf{Y}}(x_1, x_2, \overline{y}_1, \overline{y}_2, \overline{y}_3, \overline{y}_4) = \{(y_1, y_2, y_3, y_4) \in \mathbb{R}_+^4 : y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2, \ -y_1 + y_4 \le 0.8x_1 + 0.8x_2, \ y_2 + y_4 \le 4x_2, -10y_1 - 10y_2 - 10y_3 - 10y_4 \le -10\overline{y}_1 - 10\overline{y}_2 - 10\overline{y}_3 - 10\overline{y}_4\}$. *By solving its single level reformulation in the form of that in Corollary 8, we obtain an optimal solution* $x_1^* = 0$ *and* $x_2^* = 5$.

Finally, we provide a demonstration on computing the strong-weak bilevel problem.

Example 5. *Consider the following instance of the strong-weak bilevel problem, which has been solved by iterative algorithms developed in [12, 31].*

$$\min \quad -8x_1 - 6x_2 + \beta f_1 + (1 - \beta) f_2$$

$$\text{s.t.} \quad x_1 + x_2 \le 10, \ x_1, x_2 \ge 0$$

$$f_1 = \min\{-25y_1 - 30y_2 + 2y_3 + 16y_4 : (y_1, y_2, y_3, y_4) \in \mathbf{S}(x_1, x_2)\}$$

$$f_2 = \max\{-25y_1 - 30y_2 + 2y_3 + 16y_4 : (y_1, y_2, y_3, y_4) \in \mathbf{S}(x_1, x_2)\}$$

where $\mathbf{S}(x_1, x_2)$ *is defined as in (32-34). According to Corollary 9, its **R-PBL** model can be*

written as

$$\min \quad -8x_1 - 6x_2 + \beta f_1 + (1-\beta)f_2$$

$$\text{s.t.} \quad x_1 + x_2 \le 10, \ \overline{y}_1 + \overline{y}_2 + \overline{y}_3 + \overline{y}_4 \le 10 - x_1 - x_2, \ -\overline{y}_1 + \overline{y}_4 \le 0.8x_1 + 0.8x_2$$

$$\overline{y}_2 + \overline{y}_4 \le 4x_2, \ x_1, x_2, \overline{y}_1, \overline{y}_2, \overline{y}_3, \overline{y}_4 \ge 0$$

$$f_1 \ge -25y_1^o - 30y_2^o + 2y_3^o + 16y_4^o, \ (y_1^o, y_2^o, y_3^o, y_4^o) \in \mathbf{S}(x_1, x_2)$$

$$f_2 \ge -25y_1^p - 30y_2^p + 2y_3^p + 16y_4^p$$

$$(y_1^p, y_2^p, y_3^p, y_4^p) \in \arg\max \Big\{ -25y_1 - 30y_2 + 2y_3 + 16y_4 :$$

$$y_1 + y_2 + y_3 + y_4 \le 10 - x_1 - x_2, \ -y_1 + y_4 \le 0.8x_1 + 0.8x_2$$

$$y_2 + y_4 \le 4x_2, \ -10y_1 - 10y_2 - 10y_3 - 10y_4 \le -10\overline{y}_1 - 10\overline{y}_2 - 10\overline{y}_3 - 10\overline{y}_4,$$

$$y_1, y_2, y_3, y_4 \ge 0 \Big\}.$$

Again, we can compute its single level reformulation in the form of that in Corollary 9 to derive optimal solutions and values for different β. For instance, if β is set to 0.2, an optimal solution is with $(x_1^*, x_2^*) = (10, 0)$ and the optimal value is -80. If β is set to 0.5, an optimal solution is with $(x_1^*, x_2^*) = (0, 0)$ and the optimal value is -115. Results of both cases agree with those reported in [12, 31]. Moreover, by using the method of [31], we can easily consider a small number of values for β and depict the complete relationship between the optimal value and β.

5 Conclusion

In this paper, we mainly develop a tight relaxation of **PBL** and then design a simple scheme that helps us derive a solution being both feasible and optimal to **PBL**. We also discuss using this scheme to compute linear **PBL** and a few variants. Several numerical demonstrations on linear **PBL** instances are presented. Overall, we believe that, because this scheme has convenient interfaces to existing research on regular bilevel problems and does not involve any sophisticated theory or operations, it should be practically useful in solving pessimistic bilevel problems arising from real systems.

Appendix:

Computing The Extended Reformulation of **MIP − PBL**

We first provide the complete extended reformulation of **MIP − PBL**.

$$
\begin{aligned}
\min \quad & \mathbf{cx} + \eta : \\
\text{s.t.} \quad & \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{A}_2\mathbf{x} + \mathbf{B}_{2c}\overline{\mathbf{y}}_c + \mathbf{B}_{2d}\overline{\mathbf{y}}_d \leq \mathbf{b}_2 \\
& \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}}_c \in \mathbb{R}_+^{m_c}, \ \overline{\mathbf{y}}_d \in \mathbb{Z}_+^{m_d} \\
& \eta \geq \max \Big\{ \mathbf{d}_{1c}\mathbf{y}_c + \mathbf{d}_{1d}\mathbf{y}_d - M\mathbf{1}\mathbf{y}_a - My_f : \\
& \qquad \mathbf{B}_{2c}\mathbf{y}_c + \mathbf{B}_{2d}\mathbf{y}_d - \mathbf{I}\mathbf{y}_a \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}, \quad \mathbf{d}_{2c}\mathbf{y}_c + \mathbf{d}_{2d}\mathbf{y}_d - y_f \leq \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d \\
& \qquad \mathbf{y}_a \in \mathbf{R}_+^l, \ \mathbf{y}_c \in \mathbb{R}_+^{m_c}, \ \mathbf{y}_d \in \mathbb{Z}_+^{m_d}, y_f \in \mathbf{R}_+ \Big\}.
\end{aligned}
$$

Next, we describe a decomposition method, i.e., *the column-and-constraint generation algorithm*, to compute bilevel mixed integer program [30], with minor modifications customized for the aforementioned bilevel problem. Let UB and LB be the upper and lower bounds respectively, k be the iteration index and ϵ be the optimality tolerance. Note that in the following **MP** formulation, $\mathbf{y}_d^j$ are constants for all j.

Column-and-Constraint Generation Method for Bilevel MIP

Step 1: Set $LB = -\infty$, $UB = +\infty$, and $k = 0$.

Step 2: Solve the following master problem

$$
\mathbf{MP} : \underline{\Theta}_p^* = \mathbf{cx} + \eta
$$
$$
\begin{aligned}
\text{s.t. } & \mathbf{A}_1\mathbf{x} \leq \mathbf{b}_1, \ \mathbf{A}_2\mathbf{x} + \mathbf{B}_{2c}\overline{\mathbf{y}}_c + \mathbf{B}_{2d}\overline{\mathbf{y}}_d \leq \mathbf{b}_2 \\
& \eta \geq \mathbf{d}_{1d}\mathbf{y}_d^j + \mathbf{d}_{1c}\mathbf{y}_c^j - M\mathbf{1}\mathbf{y}_a^j - My_f^j, \quad 1 \leq j \leq k, \\
& \mathbf{B}_{2c}\mathbf{y}_c^j - \mathbf{I}\mathbf{y}_a^j \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_{2d}\mathbf{y}_d^j, \ 1 \leq j \leq k \\
& \mathbf{d}_{2c}\mathbf{y}_c^j - y_f^j \leq \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d - \mathbf{d}_{2d}\mathbf{y}_d^j, \ 1 \leq j \leq k \\
& \mathbf{B}_{2c}^t\mathbf{u}^j + \mathbf{d}_{2c}^t\pi^j \geq \mathbf{d}_{1c}^t, \ \mathbf{I}\mathbf{u}^j \leq M\mathbf{1}^t, \ \pi^j \leq M, \quad 1 \leq j \leq k \\
& (\mathbf{y}_c^j, \mathbf{y}_a^j, y_f^j) \perp (\mathbf{B}_{2c}^t\mathbf{u}^j + \mathbf{d}_{2c}^t\pi^j - \mathbf{d}_{1c}^t, M\mathbf{1}^t - \mathbf{I}\mathbf{u}^j, M - \pi^j), \quad 1 \leq j \leq k \\
& (\mathbf{u}^j, \pi^j) \perp (\mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_{2d}\mathbf{y}_d^j - \mathbf{B}_{2c}\mathbf{y}_c^j + \mathbf{I}\mathbf{y}_a^j, \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d - \mathbf{d}_{2d}\mathbf{y}_d^j - \mathbf{d}_{2c}\mathbf{y}_c^j + y_f), \ 1 \leq j \leq k \\
& \mathbf{x} \in \mathbb{R}_+^{n_c} \times \mathbb{Z}_+^{n_d}, \overline{\mathbf{y}}_c \in \mathbb{R}_+^{m_c}, \overline{\mathbf{y}}_d \in \mathbb{Z}_+^{m_d}; \\
& \mathbf{y}_c^j \in \mathbb{R}_+^{m_c}, \mathbf{y}_a^j \in \mathbb{R}_+^l, y_f^j \in \mathbb{R}_+, \mathbf{u}^j \in \mathbb{R}_+^l, \pi^j \in \mathbb{R}_+, \ 1 \leq j \leq k.
\end{aligned}
$$

Derive an optimal solution $(\mathbf{x}^*, \overline{\mathbf{y}}_c^*, \overline{\mathbf{y}}_d^*, \mathbf{y}_c^{1*}, \mathbf{y}_a^{1*}, y_f^{1*}, \mathbf{u}^{1*}, \pi^{1*}, \ldots, \mathbf{y}_c^{k*}, \mathbf{y}_a^{k*}, y_f^{k*}, \mathbf{u}^{k*}, \pi^{k*})$, and update $LB = \underline{\Theta}_p^*$.

Step 3: If $UB - LB \leq \epsilon$, return UB and the corresponding (incumbent) solution. Terminate. Otherwise, go to Step 4.

Step 4: Solve the following lower level problem for given $(\mathbf{x}^*, \overline{\mathbf{y}}_c^*, \overline{\mathbf{y}}_d^*)$, which serves as the subproblem.

$$
\mathbf{SP}: \quad \varphi(\mathbf{x}^*, \overline{\mathbf{y}}_c^*, \overline{\mathbf{y}}_d^*) = \max \quad \mathbf{d}_{1c}\mathbf{y}_c + \mathbf{d}_{1d}\mathbf{y}_d
$$
$$
\text{s.t.} \quad \mathbf{B}_{2c}\mathbf{y}_c + \mathbf{B}_{2d}\mathbf{y}_d \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x}^*
$$
$$
\mathbf{d}_{2c}\mathbf{y}_c + \mathbf{d}_{2d}\mathbf{y}_d \leq \mathbf{d}_{2c}\overline{\mathbf{y}}_c^* + \mathbf{d}_{2d}\overline{\mathbf{y}}_d^*
$$
$$
\mathbf{y}_c \in \mathbb{R}_+^{m_c}, \ \mathbf{y}_d \in \mathbb{Z}_+^{m_d}
$$

Derive an optimal solution $(\mathbf{y}_c^*, \mathbf{y}_d^*)$, and update $UB = \min\{UB, \mathbf{cx}^* + \varphi(\mathbf{x}^*, \overline{\mathbf{y}}_c^*, \overline{\mathbf{y}}_d^*)\}$.

Step 5: Set $\mathbf{y}_d^{k+1} = \mathbf{y}_d^*$, create variables $(\mathbf{y}_c^{k+1}, \mathbf{y}_a^{k+1}, y_f^{k+1}, \mathbf{u}^{k+1}, \pi^{k+1})$, and add the following constraints to **MP**. Set $k = k+1$ and go to Step 2.

$$
\eta \geq \mathbf{d}_{1d}\mathbf{y}_d^{k+1} + \mathbf{d}_{1c}\mathbf{y}_c^{k+1} - M\mathbf{1}\mathbf{y}_a^{k+1} - My_f^{k+1}
$$
$$
\mathbf{B}_{2c}\mathbf{y}_c^{k+1} - \mathbf{I}\mathbf{y}_a^{k+1} \leq \mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_{2d}\mathbf{y}_d^{k+1}
$$
$$
\mathbf{d}_{2c}\mathbf{y}_c^{k+1} - y_f^{k+1} \leq \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d - \mathbf{d}_{2d}\mathbf{y}_d^{k+1}
$$
$$
\mathbf{B}_{2c}^t\mathbf{u}^{k+1} + \mathbf{d}_{2c}^t\pi^{k+1} \geq \mathbf{d}_{1c}^t, \ \mathbf{I}\mathbf{u}^{k+1} \leq M\mathbf{1}^t, \ \pi^{k+1} \leq M
$$
$$
(\mathbf{y}_c^{k+1}, \mathbf{y}_a^{k+1}, y_f^{k+1}) \perp (\mathbf{B}_{2c}^t\mathbf{u}^{k+1} + \mathbf{d}_{2c}^t\pi^{k+1} - \mathbf{d}_{1c}^t, M\mathbf{1}^t - \mathbf{I}\mathbf{u}^{k+1}, M - \pi^{k+1})
$$
$$
(\mathbf{u}^{k+1}, \pi^{k+1}) \perp (\mathbf{b}_2 - \mathbf{A}_2\mathbf{x} - \mathbf{B}_{2d}\mathbf{y}_d^{k+1} - \mathbf{B}_{2c}\mathbf{y}_c^{k+1} + \mathbf{I}\mathbf{y}_a^{k+1}, \mathbf{d}_{2c}\overline{\mathbf{y}}_c + \mathbf{d}_{2d}\overline{\mathbf{y}}_d - \mathbf{d}_{2d}\mathbf{y}_d^{k+1} - \mathbf{d}_{2c}\mathbf{y}_c^{k+1} + y_f)
$$
$$
\mathbf{y}_c^{k+1} \in \mathbb{R}_+^{m_c}, \mathbf{y}_a^{k+1} \in \mathbb{R}_+^l, y_f^{k+1} \in \mathbb{R}_+, \mathbf{u}^{k+1} \in \mathbb{R}_+^l, \pi^{k+1} \in \mathbb{R}_+
$$

$\square$

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