Unboundedness in Bilevel Optimization

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Abstract

Bilevel optimization has garnered growing interest over the past decade. However, little attention has been paid to detecting and dealing with unboundedness in these problems, with most research assuming a bounded high-point relaxation. In this paper, we address unboundedness in bilevel optimization by studying its computational complexity and developing algorithmic approaches to detect it. We show that deciding whether an optimistic linear bilevel problem is unbounded is strongly NP-complete. Furthermore, we extend the theoretical intractability result to the multilevel case, by showing that for each extra level added, the decision problem of checking unboundedness moves up a level in the polynomial hierarchy. Finally, we introduce two algorithmic approaches to determine whether a linear bilevel problem is unbounded and, if so, return a certificate of unboundedness. This certificate consists of a direction of unboundedness and corresponding bilevel feasible point. We present a short proof of concept of these algorithmic approaches on some relevant examples.

Keywords: Computational Complexity, Unbounded, Bilevel Optimization, Multilevel Optimization.

1 Introduction

Bilevel optimization is a modelling framework for hierarchical interactions between non-cooperative decision makers. This framework models a Stackelberg game [16, 19, 17] with at least two players: a leader and a follower. First, the leader makes its decision. Then, given the leader's decision, the follower reacts optimally according to its own possibly-conflicting objective. In turn, the reaction of the follower influences the objective that the leader can realise. Hence, the leader must anticipate the follower's behaviour in order to accurately

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optimize its objective. Mathematically, a bilevel problem is an optimization model where some of the variables, corresponding to the follower's decisions, are constrained to be optimal for another optimization problem. This type of mathematical models with optimization problems in the constraints were first formulated in [5].

Background. Bilevel problems are known to be challenging to solve. For instance, mixed-integer bilevel problems are shown to be Σ_2^p-hard in [12]. In fact, even in their simplest form with linear objective functions and constraints, bilevel problems are strongly NP-hard [10]. In this paper, we focus on this linear case of bilevel problems, whose optimistic formulation is expressed in (B):

$$\min_{x,y} \quad c^\top x + d^\top y \tag{B.1}$$

$$\text{s.t.} \quad Ax + By \leq a \tag{B.2}$$

$$y \in \arg\min_{\tilde{y}} \quad f^\top \tilde{y} \tag{B.3}$$

$$\text{s.t.} \quad Cx + D\tilde{y} \leq b, \tag{B.4}$$

where A, B, C, D, a, b, c, d, f are matrices and vectors of rational numbers of appropriate dimension. The decision problem of the leader (B.1)-(B.2) is called the upper-level, and that of the follower (B.3)-(B.4) is the lower-level problem. The upper- and lower-level decision variables are denoted x and y, respectively, and the feasible region (B.2)-(B.4) is often referred to as inducible region.

The links between linear bilevel and mixed-integer optimization have long been the topic of research. In fact, Audet et al. [2] showed in 1997 that a binary variable $x \in \{0, 1\}$ can be modeled by the constraints $y = 0$, $0 \leq x \leq 1$, and the linear continuous problem:

$$y \in \arg\max_{\tilde{y}}\{\tilde{y} : \tilde{y} \leq x,\ \tilde{y} \leq 1 - x\}.$$

Thus showing that 0-1 linear optimization problems are a special case of linear bilevel problems. Given this connection, it should come as no surprise that the inducible region is, in general, non-convex [3], and it might even be disconnected [1, 7] in the presence of linking constraints (also known as coupling constraints), this is if $B \neq \vec{0}$.

Due to the inherent complexity of bilevel models, many bilevel solution approaches start by solving a simpler single-level relaxation. The most common relaxation is the high-point relaxation (HPR) which is obtained by simply optimizing the upper-level objective over the shared constraint set of upper- and lower-level constraints ($\mathcal{F}_{\text{HPR}}$):

$$\min_{x,y} \left\{c^\top x + d^\top y : (B.2), (B.4)\right\}. \tag{HPR}$$

It is known that, if an optimal solution of the bilevel exists, it can be found at a vertex of this relaxation's feasible set [3], which hints at the relevance of the HPR in bilevel optimization. Nevertheless, if this relaxation is unbounded, nothing can be concluded about the optimality status of the corresponding bilevel. The examples in [13] show that when the HPR model is unbounded, the corresponding bilevel can be finite optimal, unbounded, or infeasible. Due to this inconclusiveness, most bilevel solution approaches assume that the feasible set of the HPR is bounded. Consequently, there is little existing research on how to handle bilevel problems when this relaxation is unbounded.

Unboundedness. The majority of progress in the study of unbounded HPR models is made under the assumption that this unboundedness originates in the lower-level problem alone. In fact, if there is a feasible upper-level solution such that the corresponding lower-level problem is unbounded, then the bilevel problem is infeasible [22]. This key theorem has driven most of the results in this field. Note that this result is derived for mixed-integer linear bilevel problems, but it can be easily adapted to linear bilevel problems. The same holds true for the following surveyed results.

In [22], a mixed-integer linear problem is designed to track the reason for the unboundedness of the HPR, under the assumption that upper-level variables are bounded. Depending on the optimal objective value of this mixed-integer problem, we can conclude whether the bilevel is infeasible, unbounded, or finite optimal [22] (see Example 2 for an unbounded bilevel model with bounded upper-level variables). Furthermore, it is shown in [8] that, when the HPR is unbounded, one can detect whether the lower-level problem is unbounded by solving a linear problem. Depending on the optimal value of this model, we can conclude that either the bilevel is infeasible or the lower-level problem is well-defined for every feasible point of the HPR. Nevertheless, when the HPR is unbounded, but the lower-level problem is not unbounded, solving this linear model will not allow us to determine the status of the original bilevel.

Contributions. To sum up, studying the conclusions that can be drawn about the bilevel problem when its relaxation is unbounded is a relevant but often overlooked topic. In this paper, we present results aimed at closing this gap. In Section 2, we show that the decision problem of whether a linear bilevel problem is unbounded is strongly NP-complete, and make some parallels to the pessimistic bilevel formulation. More generally, we also show that checking unboundedness of a multilevel problem with k levels is Σ^p_{k-1}-hard in Section 2.3. In Section 3, we detail two possible algorithmic approaches for checking whether a bilevel problem is unbounded and, if so, computing a certificate of unboundedness. We also depict the potential of these algorithms for some example instances of interest. Finally, in Section 4 we propose directions for future research.

2 Computational Complexity of Checking Unboundedness

2.1 Decision Problem

The decision problem of deciding whether a linear model (LP) is unbounded

$$\min_x \left\{c^\top x : Ax \leq b\right\} \tag{LP}$$

can be formulated as

$$\exists x, \Delta x \in \mathbb{Q}^n,\ \forall k \geq 0 : A(x + k\Delta x) \leq b \ \wedge \ c^\top \Delta x < 0 \ ?$$

This problem has an existential quantifier, followed by a universal quantifier, and a property that can be verified in polynomial time. Consequently, it belongs to the class Σ_2^p [20]. However, this question can be simplified into one with only an existential quantifier as:

$$\exists x, \Delta x \in \mathbb{Q}^n : Ax \leq b \ \wedge \ A\Delta x \leq 0 \ \wedge \ c^\top \Delta x < 0 \ ?$$

Therefore, this allow us to say that the problem is in NP$\subseteq \Sigma_2^p$. Furthermore, we know that we can solve a linear model in polynomial-time by applying an interior point method [23], and that such algorithm also identifies unboundedness. Thus, we can further write the question without an existential quantifier, allowing us to conclude that the problem is in P$\subseteq$ NP. It is exactly this type of reasoning that will guide our contributions when proving that the decision problem of checking unboundedness of a linear bilevel problem is in NP. But first, we formally define this decision problem.

In general, we know that an optimization problem is unbounded if it admits a feasible point, and a direction of unboundedness at that point. In turn, a direction of unboundedness must be a direction along which feasibility is preserved and the objective value improved. Therefore, we say that a direction $(\Delta x, \Delta y)$ is a direction of unboundedness at a feasible point (x, y), if it verifies:

$$(x, y) + k(\Delta x, \Delta y) \in \mathcal{F}_{\text{B}} \quad \forall k \geq 0 \tag{2}$$

$$c^\top \Delta x + d^\top \Delta y < 0 \tag{3}$$

where $\mathcal{F}_{\text{B}}$ denotes the inducible region. Consequently, we define the decision problem for whether the optimistic linear bilevel problem (B) is unbounded as UNBOUNDED-BLP.

UNBOUNDED-BLP:
INSTANCE: A, B, C, D, a, b, c, d, f matrices and vectors of rational numbers and of appropriate dimension.
QUESTION: Is the bilevel problem (B) unbounded? Equivalently, are there a feasible solution $(x, y) \in \mathcal{F}_{\text{B}}$ and a direction $(\Delta x, \Delta y)$ at that point that verify (2)-(3)?

In the following section, we show that this decision problem is strongly NP-complete, by showing that it is both in NP and strongly NP-hard.

2.2 NP-completeness of Bilevel Case

2.2.1 Inclusion in NP.

In this section, we prove that UNBOUNDED-BLP belongs to the complexity class NP. First, we present two auxiliary results that allow us to formulate the problem's question as one involving a single existential quantifier. This formulation is based on the reformulation of the inducible region as a finite union of polyhedra from [4]. For detailed proofs of these results, Lemma 1 and Theorem 1, see Appendix A.

Lemma 1. *The bilevel problem (B) is unbounded if and only if the finite-union-of-polyhedra reformulation (P) is unbounded.*

$$\min_{x,y,\lambda} \quad c^\top x + d^\top y \tag{P.1}$$

$$s.t. \quad (x,y,\lambda) \in \bigcup_{\omega \in \{1,2\}^{n_2}} \mathcal{P}_\omega \tag{P.2}$$

where λ are the dual variables of the lower-level problem, n_2 is the number of lower-level constraints, and the polyhedra $\mathcal{P}_\omega$ are defined as:

$$\begin{aligned} \mathcal{P}_\omega = \{(x,y,\lambda) \in \mathcal{F} : \ & (Cx + Dy - b)_i = 0 && \forall i : \omega_i = 1; \\ & \lambda_i = 0 && \forall i : \omega_i = 2\} \end{aligned}$$

where $\mathcal{F}$ consists of the upper- and lower-level constraints ((B.2), (B.4)), plus the lower-level dual constraints ($D^\top \lambda = -f^\top; \lambda \geq 0$).

Theorem 1. *The finite-union-of-polyhedra reformulation (P) is unbounded if and only if $\exists \omega \in \{1,2\}^{n_2}$ such that the linear problem (P_ω) is unbounded.*

$$\begin{aligned} \min_{x,y,\lambda} \ & c^\top x + d^\top y \\ s.t. \ & (x,y,\lambda) \in \mathcal{P}_\omega \end{aligned} \tag{P$_\omega$}$$

Given Lemma 1 and Theorem 1, we conclude that UNBOUNDED-BLP can be equivalently formulated as:

$$\exists\ \omega \in \{1,2\}^{n_2} : (\mathrm{P}_\omega) \text{ is unbounded?}$$

This is a formulation with a single existential quantifier, followed by the property of whether a linear problem is unbounded, which can be verified in polynomial time [23]. Therefore, this problem belongs to the complexity class NP [20]. Note that the cardinality of the set $\{1,2\}^{n_2}$ is exponential in the instance size, therefore we cannot trivially say that the problem is polynomially solvable.

2.2.2 Strong NP-hardness.

We now conclude that UNBOUNDED-BLP is strongly NP-complete in Theorem 2, by proving that it is also strongly NP-hard.

Theorem 2. UNBOUNDED-BLP *is strongly NP-complete.*

In order to prove this result, we derived a reduction from the decision version of the 3-SAT problem known to be NP-complete [9]. For a proof see Appendix A.

Remark 1 (Linking constraints)**.** *Note that while the presence of linking constraints (this is $B \neq \vec{0}$) plays an important role in the proof of strong NP-hardness, the inclusion of* UNBOUNDED-BLP *in NP is valid even for bilevel problems without linking constraints. Although it is desirable to obtain a stronger proof of NP-hardness that uses a bilevel without linking constraints in the reduction, this remains an open question. While existing work demonstrates the reformulation of bilevel problems with linking constraints into those without, these approaches rely on the assumption that the bilevel problem has a finite optimal solution [11]. Notably, one of the crucial steps in [11] is related to reformulating complementarity constraints using big-M constants by following the procedure in [6] based on the analysis of lower-level basic solutions. However, it is not clear that this can be adapted when there is a direction of unboundeness. Therefore, these ideas are not applicable to our context.*

Remark 2 (Pessimistic Formulation)**.** *So far we have considered the optimistic formulation of a linear bilevel problem. In other words, we assumed that when there are multiple optimal solutions of the lower-level problem, the follower chooses the optimal solution that benefits the leader the most. Another common formulation is the pessimistic one [14] where the opposite is assumed. In this formulation, if there are multiple lower-level optimal solutions, the worst solution with respect to the upper-level will be selected. Hence, the optimization of the upper-level objective in (B.1) is replaced with:*

$$\min_{x} \max_{\tilde{y}} \; c^\top x + d^\top \tilde{y}$$

In general, unboundedness of the optimistic formulation of a bilevel problem does not imply that of its pessimistic formulation (see Appendix B). Nevertheless, the NP-hardness part of Theorem 2 still holds if we consider a pessimistic formulation, because the lower-level variables in the reduction are uniquely defined by the upper-level variables. In other words, the pessimistic and optimistic formulations are equivalent for the bilevel problem used in the reduction. Therefore, the decision problem of whether a pessimistic linear bilevel model is unbounded is also strongly NP-hard.

2.3 Extension to Multilevel Case

In this section, we extend our results to multilevel optimization by showing that deciding whether a k-level optimization problem is unbounded is Σ^p_{k-1}-hard. We have seen that for $k = 2$, checking if a bilevel problem is unbounded is NP-hard, or equivalently Σ^p_1-hard. So this extension shows that for each level added to a multilevel problem, the complexity of deciding unboundedness moves up a level in the polynomial hierarchy. First, we introduce an optimistic k-level problem (KLP):

$$
\begin{aligned}
\min_{x} \quad & c_k^\top x \\
\text{s.t.} \quad & x \in S^k \\
& x^{(k-1)} \in \arg\min_{x^{(k-1)}} \quad c_{k-1}^\top x^{(k-1)} \\
& \qquad\qquad \text{s.t.} \quad x^{(k-1)} \in S^{k-1} \\
& \qquad\qquad\qquad x^{(k-2)} \in \arg\min_{x^{(k-2)}} \quad (\dots) \\
& \qquad\qquad\qquad\qquad \vdots \\
& \qquad\qquad\qquad x^{(2)} \in \arg\min_{x^{(2)}} \quad c_2^\top x^{(2)} \\
& \qquad\qquad\qquad\qquad \text{s.t.} \quad x^{(2)} \in S^2 \\
& \qquad\qquad\qquad\qquad\qquad x^{(1)} \in \arg\min_{x^{(1)}} \quad c_1^\top x^{(1)} \\
& \qquad\qquad\qquad\qquad\qquad\qquad \text{s.t.} \quad x^1 \in S^1
\end{aligned}
\tag{KLP}
$$

where $x = (x^1, \dots, x^k)$ are the decision variables, and S^i is the linear feasible region of level i; note the slight abuse of notation on the use of the same variable notation over different levels. The set S^i is parameterized by the variables of all the levels above i, so the notation S^i is an abbreviation for $S^i(x^{i+1}, \dots, x^k)$. The subset of decision variables of level i is $x^{(i)} = (x^1, \dots, x^i)$, and c_i the corresponding objective coefficients.

The decision problem of deciding whether the linear k-level problem (KLP) is unbounded can be stated as:

Unbounded-KLP:
instance: $c_k, \dots, c_1$ rational vectors of appropriate dimension and $S^k, \dots, S^1$ linear polyhedra (defined by rational coefficients).
question: Is the corresponding k-level model unbounded?

In Theorem 3, we show that Unbounded-KLP (with linking constraints only in its level k) is strongly Σ_{k-1}^p-hard.

Theorem 3. Unbounded-KLP *is* Σ_{k-1}^p*-hard.*

In order to prove this result, we derived a reduction from the decision version of the $(k-1)$-Alternating Quantified Satisfiability problem known to be Σ_{k-1}^p-complete [21]. For a proof see Appendix C.

3 Algorithmic Approaches

Despite the theoretical intractability of deciding whether (B) is unbounded, this section explores methods for addressing it. We present two algorithmic approaches to check whether a bilevel problem is unbounded when its HPR is. The first, a natural method leveraging on previously presented results, reduces to solving a *hard* problem. The second is more intricate and it is designed so that each step solves *easier* problems.

3.1 LPCC Reformulation

The first approach consists in reformulating our decision problem as a linear problem with complementarity constraints (LPCC). Such problems can be fed into mixed-integer linear solvers like Gurobi, where complementarity constraints are handled using SOS constraints of type 1. As shown in Theorem 4, the objective value of this LPCC allow us to conclude whether the corresponding bilevel problem is unbounded. For a complete proof of Theorem 4 see Appendix D.

Theorem 4. *The bilevel problem (B) is unbounded if and only if the LPCC (U) has strictly negative optimal value.*

$$
\begin{aligned}
\min_{x,y,\lambda,\Delta x,\Delta y} \quad & c^\top \Delta x + d^\top \Delta y && \text{(U.1)}\\
s.t. \quad & (x,y,\lambda) \in \mathcal{F} && \text{(U.2)}\\
& (Cx + Dy - b)\lambda = 0 && \text{(U.3)}\\
& A\Delta x + B\Delta y \le 0 && \text{(U.4)}\\
& C\Delta x + D\Delta y \le 0 && \text{(U.5)}\\
& (C\Delta x + D\Delta y)\lambda = 0 && \text{(U.6)}\\
& -1 \le \Delta x, \Delta y \le 1 && \text{(U.7)}
\end{aligned}
$$

where once again $\mathcal{F} = \big\{(x,y,\lambda) : (B.2);\ (B.4);\ D^\top\lambda = -f^\top;\ \lambda \ge 0\big\}$. *Moreover, when an optimal solution exists, its component* (x,y) *provides a feasible point and its component* $(\Delta x, \Delta y)$ *a direction of unboundedness at* (x,y).

Note that, from the optimization status and optimal value of the problem (U), we can extract further conclusions about the corresponding bilevel problem (B). The problem (U) cannot be unbounded, because of constraint (U.7). When (U) is infeasible, so is the bilevel problem (B). We know this because $(\Delta x, \Delta y) = (\vec{0}, \vec{0})$ is always feasible for (U), so infeasibility of this model reveals that there is no bilevel feasible point (x,y,λ). When (U) is finite optimal, we know that its optimal value is non-positive. On the one hand, if the optimal value is strictly negative, Theorem 4 allows us to conclude that the bilevel problem is unbounded. On the other hand, if the optimal value is zero, then we know that the bilevel problem (B) is finite optimal, since it is feasible and not unbounded.

Remark 3 (Dual Component of Direction of Unboundedness)**.** *Note that the model* (U) *does not consider the component of the direction in the lower-level dual space* ($\Delta\lambda$)*. In fact, as evidenced in the proof of Theorem 4, if* $(\Delta x, \Delta y)$ *is a direction of unboundedness for the bilevel, we can always trivially extend it to the lower-level dual space with* $\Delta\lambda$=0*. Indeed, in case of unboundedness, under the optimal solution* $(x^\star, y^\star, \lambda^\star, \Delta x^\star, \Delta y^\star)$ *of* (U)*, for all* $k \ge 0$, $y^\star + k\Delta y^\star$ *is an optimal solution of the lower-level problem at* $x = x^\star + k\Delta x^\star$*, where the basis (for the lower-level problem) is always the same. Hence, the associated dual optimal solution does not change.*

3.2 Vertex-Enumeration Algorithm

The second approach is a vertex-enumeration algorithm detailed in Algorithm 1. The idea behind this algorithm is that given a bilevel feasible point, we can check all directions of unboundedness of the HPR at this point (step 5) for whether they are also directions of unboundedness of the bilevel problem (B) by solving a linear problem. In fact, we verify whether a given direction generates unboundedness for the bilevel problem, by determining whether it has associated dual values, hence ensuring it belongs to a polyhedron $\mathcal{P}_\omega$ (steps 7 and 8).

Algorithm 1: Vertex-Enumerating Algorithm

1 **for** *$\mathcal{B}$ set of basic indexes of $\mathcal{F}_{HPR}$* **do**
2   **if** *$\mathcal{B}$ yields a basic feasible solution (v_x, v_y) of $\mathcal{F}_{HPR}$* **then**
3   **if** *(v_x, v_y) is bilevel feasible* **then**
4   Compute the reduced costs $\bar{c}$ and constraint matrix coefficients $\bar{A}$ in the simplex tableau of (HPR) at (v_x, v_y);
5   **for** *i variable index with $\bar{c}_i < 0$ and $\bar{A}_{\cdot,i} \leq \mathbf{0}$ and $\bar{A}_{\cdot,i} \neq \mathbf{0}$* **do**
6   Set $(\Delta v_x, \Delta v_y)$ equal to $-\bar{A}_{\cdot,i}$ for basic variables in $\mathcal{B}$, 1 for variable i, and 0 for non-basic variables;
7   With $(x, y, \Delta x, \Delta y) = (v_x, v_y, \Delta v_x, \Delta v_y)$ fixed, solve (U') : $\min_{\lambda \geq 0} \left\{0 : D^\top \lambda = -f^\top; (U.3); (U.6)\right\}$;
8   **if** *(U') is feasible* **then**
9   **return** $(v_x, v_y, \Delta v_x, \Delta v_y)$
10 **return** $(\{\}, \{\}, \{\}, \{\})$ `// (B) is bounded (optimal or infeasible)`

In order to ensure the correctness of this algorithmic approach, we show two results. First, Lemma 2 establishes that it is enough to search for directions of unboundedness of (B) at the basic feasible solutions (i.e. vertices) of the HPR's feasible set. For this result to hold, we assume that the HPR's feasible set has at least one vertex. This can be verified through checking that:

$$\text{span}\left\{[A_i|B_i]_{i\in\{1,\ldots,n_1\}}, [C_j|D_j]_{j\in\{1,\ldots,n_2\}}\right\} = \mathbb{R}^{n_1+n_2}$$

where n_1 and n_2 are the number of upper- and lower-level constraints, respectively. Note also that this property holds valid for any problem in standard form (i.e. with non-negativity constraints).

Lemma 2. *The bilevel problem (B) is unbounded if and only if there exists a feasible point $(x', y') \in \mathcal{F}_B$ and a direction of unboundedness $(\Delta x', \Delta y')$ of (B) such that (x', y') is a vertex of the HPR's feasible set.*

Proof. The statements about the existence of a feasible point and direction of unboundedness follow naturally from the definition of an unbounded bilevel problem (recall (2)-(3)). Therefore, the indirect implication follows naturally.

For the direct implication, we show that at least one bilevel feasible point where there is a direction of unboundedness is a vertex of the HPR's feasible set. Assume the bilevel problem (B) is unbounded. From Lemma 1 and Theorem 1, we have that there exists $\omega \in \{1,2\}^{n_2}$ such that (P_ω) is unbounded. Let $(\Delta x', \Delta y', \Delta\lambda')$ be a direction of unboundedness of that linear problem. Then $(\Delta x', \Delta y')$ is a direction of unboundedness of the bilevel problem (B) (see proofs of Lemma 1 and Theorem 1 for further details).

Furthermore, we know that the feasible region of (P_ω) has a vertex, because by assumption the $\mathcal{F}_{\text{HPR}}$ has a vertex and the extra variables λ are non-negative. Let (x', y', λ') be that vertex, at which we know the direction $(\Delta x', \Delta y', \Delta\lambda')$ holds because (P_ω) is a linear problem. By construction, if (x', y', λ') is a vertex of (P_ω), then (x', y') is a vertex of the HPR's feasible set (see Appendix E for a proof). Therefore, there is a bilevel feasible point (x', y') which is a vertex of the HPR's feasible set, and for which there is a direction of unboundedness $(\Delta x', \Delta y')$ for the bilevel problem.

□

The next Lemma 3 shows that we can restrict the search for a direction of unboundedness for (B) to extreme rays of the HPR.

Lemma 3. *In step 7 of Algorithm 1, there exists v_λ feasible to (U') if and only if $(\Delta v_x, \Delta v_y)$ is a direction of unboundedness of the bilevel at (v_x, v_y).*

Proof. It is possible to observe that, given (v_x, v_y) a bilevel feasible point and $(\Delta v_x, \Delta v_y)$ a direction of unboundedness of the HPR at (v_x, v_y), v_λ is a solution of (U') if and only if $(v_x, v_y, v_\lambda, \Delta v_x, \Delta v_y)$ is a solution of (U). Moreover, since $(\Delta v_x, \Delta v_y)$ is a direction of unboundedness of the HPR, then $c^\top \Delta v_x + d^\top \Delta v_y < 0$. Thus, from Theorem 4, we have that there is a feasible solution of (U') if and only if $(\Delta v_x, \Delta v_y)$ is a direction of unboundedness of the bilevel at (v_x, v_y). □

The preceding Lemmas 2 and 3 along with the fact that the HPR has a finite number of bases and that step 5 involves a finite number of possible rays for the HPR, lead us to the conclusion that:

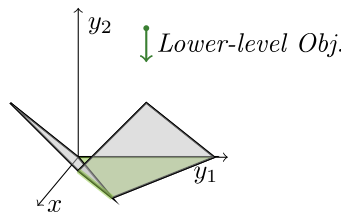
Theorem 5. *Algorithm 1 determines in a finite number of steps whether* (B) *is unbounded, and if so, it returns a certificate of unboundedness. This certificate consists of a bilevel feasible point and a direction of boundedness at that point.*

3.3 Insights from Illustrative Examples

We illustrate the behavior of these two algorithmic approaches, the LPCC reformulation and the vertex-enumeration Algorithm 1, on two examples of unbounded bilevel problems. An example of a bounded bilevel with an unbounded HPR can be found in Appendix F.

Example 1 (Book Spine)**.** *Consider the unbounded bilevel model below and the corresponding graph, where the bilevel feasible region is colored green, and the direction is that of improving lower-level objective.*

$$
\begin{aligned}
\max_{x \geq 0, y_1, y_2} \quad & y_2 \\
s.t. \quad & (y_1, y_2) \in \quad \arg\min_{\tilde{y_1}, \tilde{y_2} \geq 0} \{\tilde{y}_2 : \\
& \qquad\qquad x + \tilde{y}_1 - \tilde{y}_2 \leq 2 \\
& \qquad\qquad x - \tilde{y}_1 - \tilde{y}_2 \leq 0\}.
\end{aligned}
$$



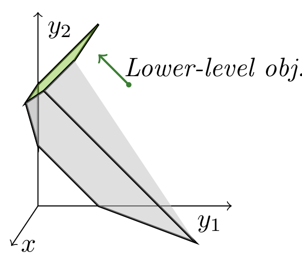
In this example the sequence of points leading to unboundedness of the bilevel lays on the intersection of two lower-level facets, this is along the "book spine". There is not a single lower-level facet that is unbounded (and bilevel feasible), but rather the intersection of two facets. In addition, for $x \in [0, 1[$, there are multiple lower-level optimal solutions (green area where $y_2 = 0$).

Both the LPCC (U) and the vertex-enumeration Algorithm 1 reveal the direction of unboundedness $(\Delta x, \Delta y_1, \Delta y_2) = (1, 0, 1)$ at the bilevel feasible point $(x, y_1, y_2) = (1, 1, 0)$. In our implementation, the vertex-enumeration algorithm performed 8 iterations, exploring 8 possible bases of the HPR. In the last iteration, it found the basic feasible solution associated with the vertex $(x, y_1, y_2) = (1, 1, 0)$, where the basic variables are x and y_1. In its simplex tableaux, the non-basic variable y_2 has a negative reduced cost of $\bar{c}_i = -1$, and a non-positive nonzero column $\bar{A}_{\cdot,i} = [-1\ 0]^\top$. According to step 6, the direction of unboundedness for the HPR is built as $(\Delta x, \Delta y_1, \Delta y_2) = (1, 0, 1)$. The model (U') is solved for this direction and for $(x, y_1, y_2) = (1, 1, 0)$ fixed, and a lower-level dual solution $(\lambda_1, \lambda_2) = (\frac{1}{2}, \frac{1}{2})$ is found. Thus, the algorithm concludes correctly that the bilevel problem is unbounded.

An example of a basis which yields a basic feasible solution where there is a direction of unboundedness for the HPR, but not for the bilevel is the one containing both lower-level slack variables. This basis yields the HPR basic feasible solution associated with the vertex $(x, y_1, y_2) = (0, 0, 0)$ which is also bilevel optimal. According to step 6, a direction of unboundedness for the HPR can be built as $(\Delta x, \Delta y_1, \Delta y_2) = (0, 0, 1)$. However, in this case the model (U') is infeasible. From constraints (U.6), we have that both dual variables λ_1 and λ_2 are forced to be 0. However, the dual constraint associated with y_2, states that $-\lambda_1 - \lambda_2 = -1$. These simultaneous restrictions on λ_1 and λ_2 deem the problem (U') infeasible. Thus, Algorithm 1 discards this basis, and keeps searching.

Example 2 (Bounded Upper-level Variables)**.** *Consider the unbounded bilevel model below and the corresponding graph, where the bilevel feasible region is colored green, and the direction is that of improving lower-level objective.*

$$
\begin{aligned}
\min_{x \geq 0, y_1, y_2} \quad & x - y_1 \\
s.t. \quad & x \leq 2 \\
& (y_1, y_2) \in \quad \arg\min_{\tilde{y_1}, \tilde{y_2} \geq 0} \{\tilde{y}_1 - \tilde{y}_2 : \\
& \qquad\qquad -y_1 + y_2 \leq 2 \\
& \qquad\qquad x - y_1 - y_2 \leq -1\}.
\end{aligned}
$$



This example is relevant because even though the upper-level variables x are bounded, and the lower-level problem is finite optimal for each feasible value of x, the bilevel is unbounded. This is possible, because for fixed variables x, the lower-level is bounded (with respect to the lower-level objective), but has an infinite number of optimal solutions that form a sequence which is unbounded with respect to the upper-level objective.

Both the LPCC (U) and the vertex-enumeration Algorithm 1 confirm that $(\Delta x, \Delta y_1, \Delta y_2) = (0, 1, 1)$ *is a direction of unboundedness at the bilevel feasible point* $(x, y_1, y_2) = (0, 0, 2)$. *In our implementation, the vertex-enumeration algorithm performed 26 iterations, by exploring 26 possible bases of the HPR. In the last iteration, it found the basic feasible solution associated with the vertex* $(x, y_1, y_2) = (0, 0, 2)$, *where the basic variables are* y_2 *and the slack variables of the constraints* ($x \leq 2$) *and* ($x - y_1 - y_2 \leq -1$). *In its simplex tableaux, the non-basic variable* y_1 *has a negative reduced cost of* $\bar{c}_i = -1$, *and a non-positive nonzero column* $\bar{A}_{\cdot,i} = [-1 \ 0 \ -2]^\top$. *According to step 6, we build a direction of unboundedness for the HPR as* $(\Delta x, \Delta y_1, \Delta y_2) = (0, 1, 1)$ *(and* $(0, 0, 2)$ *for the three slack variables). Finally, the model (U') is solved for this direction and for* $(x, y_1, y_2) = (1, 1, 0)$ *fixed, and a lower-level dual solution* $(\lambda_1, \lambda_2) = (1, 0)$ *is found. Thus, the algorithm concludes correctly that the bilevel problem is unbounded, and* $(\Delta x, \Delta y_1, \Delta y_2) = (0, 1, 1)$ *is a direction of unboundedness at the bilevel feasible point* $(x, y_1, y_2) = (0, 0, 2)$.

4 Future Work

We presented results aimed at dealing with the often-overlook topic of unboundedness in bilevel optimization. Future research could focus on deriving the computational complexity of deciding whether an optimistic linear bilevel problem without linking constraints is unbounded. Additionally, the complexity results could also be further extended to mixed-integer or multi-follower bilevel problems. A more exhaustive computational experience comparing the performance of the two algorithmic approaches proposed is also warranted. While the LPCC approach requires solving an NP-hard problem, Algorithm 1 solves a series of systems of linear constraints. However, if the bilevel problem (B) is bounded (and its HPR unbounded), we must enumerate all basic feasible solutions of the HPR. Thus, in this case, it would be worth saving the best bilevel feasible solution along Algorithm 1, so that we are also able to return the optimal solution. Furthermore, developing heuristics to prioritize the enumeration of vertices of the HPR that lay on lower-level faces which are unbounded for this relaxation may enhance the algorithm's efficiency in proving unboundedness. Finally, designing a diverse bilevel dataset would be desirable, as existent ones mostly have instances with a bounded HPR [18].

References

[1] Charles Audet, Jean Haddad, and Gilles Savard. A note on the definition of a linear bilevel programming solution. *Applied Mathematics and Computation*, 181(1):351–355, 2006.

[2] Charles Audet, Pierre Hansen, Brigitte Jaumard, and Gilles Savard. Links between linear bilevel and mixed 0–1 programming problems. *Journal of optimization theory and applications*, 93:273–300, 1997.

[3] Jonathan F. Bard. *Practical Bilevel Optimization*, volume 30. Springer US, Boston, MA, 1998.

[4] Amitabh Basu, Christopher Thomas Ryan, and Sriram Sankaranarayanan. Mixed-Integer Bilevel Representability. *Mathematical Programming*, 185(1-2):163–197, 2021.

[5] Jerome Bracken and James T McGill. Mathematical Programs with Optimization Problems in the Constraints. *Operations Research*, 21(1):37–44, 1973.

[6] Christoph Buchheim. Bilevel linear optimization belongs to NP and admits polynomial-size KKT-based reformulations. *Operations Research Letters*, 51(6):618–622, 2023.

[7] Benoît Colson, Patrice Marcotte, and Gilles Savard. An overview of bilevel optimization. *Annals of Operations Research*, 153(1):235–256, 2007.

[8] Matteo Fischetti, Ivana Ljubić, Michele Monaci, and Markus Sinnl. On the Use of Intersection Cuts for Bilevel Optimization. *Mathematical Programming*, 172(1-2):77–103, 2018.

[9] Michael R. Garey and David S. Johnson. *Computers and intractability : a guide to the theory of NP-completeness*. A Series of books in the mathematical sciences. W.H. Freeman, New York, 1979.

[10] Pierre Hansen, Brigitte Jaumard, and Gilles Savard. New Branch-and-Bound Rules for Linear Bilevel Programming. *SIAM Journal on Scientific and Statistical Computing*, 13(5):1194–1217, 1992.

[11] Dorothee Henke, Henri Lefebvre, Martin Schmidt, and Johannes Thürauf. On Coupling Constraints in Linear Bilevel Optimization. *arXiv preprint*, 2024.

[12] Robert G. Jeroslow. The polynomial hierarchy and a simple model for competitive analysis. *Mathematical Programming*, 32(2):146–164, 1985.

[13] Thomas Kleinert, Martine Labbé, Ivana Ljubić, and Martin Schmidt. A Survey on Mixed-Integer Programming Techniques in Bilevel Optimization. *EURO Journal on Computational Optimization*, 9:100007, 2021.

[14] June Liu, Yuxin Fan, Zhong Chen, and Yue Zheng. Pessimistic Bilevel Optimization: A Survey. *International journal of computational intelligence systems*, 11(1):725–736, 2018.

[15] Patrice Marcotte and Gilles Savard. Bilevel programming: A combinatorial perspective. In *Graph theory and combinatorial optimization*, pages 191–217. Springer, 2005.

[16] Heinrich von Stackelberg. *Marktform und gleichgewicht*. Springer, 1934.

[17] Stackelberg, Heinrich von. *Market Structure and Equilibrium*. Springer Berlin, Heidelberg, 1 edition, 2011.

[18] Johannes Thürauf, Thomas Kleinert, Ivana Ljubić, Ted Ralphs, and Martin Schmidt. BOBILib: Bilevel Optimization (Benchmark) Instance Library, 2024.

[19] Heinrich Von Stackelberg, Alan T Peacock, Erich Schneider, and TW Hutchison. The theory of the market economy. *Economica*, 20(80):384, 1953.

[20] Woeginger, Gerhard J. The trouble with the second quantifier. *4OR*, 19(2):157–181, 2021.

[21] Celia Wrathall. Complete sets and the polynomial-time hierarchy. *Theoretical Computer Science*, 3(1):23–33, 1976.

[22] Pan Xu and Lizhi Wang. An Exact Algorithm for the Bilevel Mixed Integer Linear Programming Problem Under Three Simplifying Assumptions. *Computers & Operations Research*, 41:309–318, 2014.

[23] Yinyu Ye, Michael J Todd, and Shinji Mizuno. An O($\sqrt{n}$L)-Iteration Homogeneous and Self-Dual Linear Programming Algorithm. *Mathematics of operations research*, 19(1):53–67, 1994.

A Auxiliary Results for NP-Completeness

In this appendix, we present the detailed proofs of Lemma 1 and Theorems 1 and 2. First, Lemma 1 states that the bilevel problem (B) is unbounded if and only if the finite-union-of-polyhedra reformulation (P) is unbounded. Its proof follows.

Lemma 1. From [4, Theorem 8], we know that the set of linear bilevel representable feasible regions is equivalent to a set of finite unions of polyhedra. In particular, the proof of this result is constructive, showing that by applying the KKT conditions to the lower level of (B), we obtain the equivalent set (P). In other words, there is a linear transformation between the points in the feasible sets of problems (B) and (P).

If the bilevel problem (B) is unbounded, then there exists a sequence of feasible points $\{(x_i, y_i)\}_{i\in\mathbb{Z}^+}$ with decreasing upper-level objective value. Applying the linear transformation between (B) and (P), which we know exists from [4], we obtain a sequence of points $\{(x_i, y_i, \lambda_i)\}_{i\in\mathbb{Z}^+}$ feasible for problem (P) with decreasing (upper-level) objective value. Therefore, we conclude that the problem (P) is unbounded. A similar argument can be used to show the opposite implication, hence proving that the problem (B) is unbounded if and only if the reformulation (P) is unbounded. □

Second, we present the proof of Theorem 1 which states that the finite-union-of-polyhedra reformulation (P) is unbounded if and only if there exists an $\omega \in \{1,2\}^{n_2}$ such that the linear problem (P$_\omega$) is unbounded.

Theorem 1. If $\exists \omega \in \{1,2\}^{n_2}$ such that (P$_\omega$) is unbounded, then (P) is also unbounded, because (P) is a relaxation of (P$_\omega$).

To prove the opposite implication, we assume that (P) is unbounded and, by contradiction, that for all $\omega \in \{1,2\}^{n_2}$ (P$_\omega$) is not unbounded (i.e., it is either infeasible or finite optimal). Consequently, we have that $\forall \omega \in \{1,2\}^{n_2}$ $\exists L_\omega \in \mathbb{R} \cup \{+\infty\}$ such that:

$$\forall (x, y, \lambda) \in \mathcal{P}_\omega : \ c^\top x + d^\top y \geq L_\omega.$$

where the convention is that $L_\omega = +\infty$ corresponds to an infeasible problem. Note that since (P) is feasible, we know that at least one of these bounds $L_\omega \in \mathbb{R}$ is finite. Therefore, we know that:

$$\forall (x, y, \lambda) \in \bigcup_{\omega\in\{1,2\}^{n_2}} \mathcal{P}_\omega : \ c^\top x + d^\top y \geq \min_{\omega\in\{1,2\}^{n_2}} \{L_\omega\} \in \mathbb{R}$$

which contradicts the assumption that (P) is unbounded. Hence, if (P) is unbounded, then $\exists \omega \in \{1,2\}^{n_2}$ such that (P$_\omega$) is unbounded. We have proved both implications as required. □

Lastly, we present the proof of Theorem 2 which states that the decision problem Unbounded-BLP is strongly NP-complete.

First, we present the decision version of the 3-SAT problem known to be NP-complete [9] which we use in the reduction proof.

3-Satisfiability (3-SAT): INSTANCE: S set of m clauses on the boolean variables $\{a_i\}_{i\in\{1,\dots,n\}}$, each clause with at most 3 literals QUESTION: Is there a true/false assignment of the boolean variables a_i such that S is satisfied?

Following the notation used in [15], S is satisfiable if an only if there exists $a \in \{0,1\}^n$ such that $A_{\text{S}}a \geq 1 + c_{\text{S}}$, where $A_{\text{S}} \in \{-1,0,1\}^{m\times n}$ and $c_{\text{S}} \in \{-3,-2,-1,0\}^m$. Based on this rewriting of 3-SAT, we prove Theorem 2 which states that Unbounded-BLP is a strongly NP-complete problem.

Theorem 2. From Lemma 1 and Theorem 1, we concluded that Unbounded-BLP is in NP. It remains to show that it is (strongly) NP-hard. We achieve this by showing that (3-SAT) is a YES instance if and only if the bilevel model (B') is unbounded.

$$\max_{x,y,z} \Big\{ y : A_{\text{S}}x \geq (1+c_{\text{S}})y; \quad 0 \leq x_i \leq y \ \forall i \in \{1,\dots,n\}; \qquad y \geq 1; \quad z = \vec{0}; \quad z \in \phi(x,y) \Big\}, \tag{B'}$$

where $\phi(x,y) = \arg\max_{\bar{z}\geq 0} \left\{ \sum_{i=1}^{n} \bar{z}_i : \bar{z}_i \leq x_i; \ \bar{z}_i \leq y - x_i \ \forall i \in \{1,\dots,n\} \right\}.$

Proof of if. If (3-SAT) is a YES instance, then $\exists a \in \{0,1\}^n : \ A_{\text{S}}a \geq (1+c_{\text{S}})$. Consequently, we build a bilevel feasible solution of (B') with $(x^*,y^*,z^*) = (a,1,\vec{0})$, and a direction of unboundedness with $(\Delta x, \Delta y, \Delta z) = (a,1,\vec{0})$. Hence, (B') is unbounded.

Proof of only if. If 3-SAT is a NO instance, then there is no $a \in \{0,1\}^n$ such that $A_{\text{S}}a \geq 1 + c_{\text{S}}$. Thus, any feasible $a \in [0,1]^n$ for $A_{\text{S}}a \geq 1 + c_{\text{S}}$ implies that $\exists i : a_i \in]0,1[$.

We remark that due to the linking constraint $z_i = 0$, any bilevel feasible solution must have $x \in \{0,y\}^n$. Moreover, since $y \geq 1$, we can write:

$$A_{\text{S}}x \geq (1+c_{\text{S}})y \Leftrightarrow A_{\text{S}}\frac{x}{y} \geq 1 + c_{\text{S}}.$$

This makes it clear that *(i)* any upper-level feasible (x,y) can be map onto $a = \frac{x}{y} \in [0,1]^n$ such that $A_{\text{S}}a \geq 1 + c_{\text{S}}$ and *(ii)* any $a \in [0,1]^n$ such that $A_{\text{S}}a \geq 1 + c_{\text{S}}$ can be mapped onto an infinite set of upper-level feasible solutions of the form $(x,y) = (a \cdot y, y) \ \forall y \geq 1$. Given that S is a NO instance, this reasoning implies that any upper-level feasible solution has some $x_i \in]0,y[$. However, this results in $\bar{z}_i = \min\{x_i, y - x_i\} > 0$ which is infeasible for the upper-level linking constraint $z = \vec{0}$. Hence, (B') is not unbounded. □

B Unboundedness in Optimistic vs. Pessimistic Bilevel Optimization

In this section, we show an example illustrating why unboundedness of the optimistic formulation does not imply that of the pessimistic formulation.

Consider the following bilevel problem:

$$\begin{array}{lll} \min\limits_{"x"} & -x + y_1 - y_2 & \\ \text{s.t.} & (y_1, y_2) \in \arg\min\limits_{\tilde{y}_1, \tilde{y}_2} & -\tilde{y}_1 - \tilde{y}_2 \\ & \qquad\qquad\qquad\qquad \text{s.t.} & -x + \tilde{y}_1 + \tilde{y}_2 \leq 1 \\ & & \tilde{y}_1, \tilde{y}_2 \geq 0 \ , \end{array}$$

where the upper-level is purposefully ill-defined, because we will consider both the optimistic and the pessimistic versions of the problem in this section.

The lower-level constraints imply that any feasible x must be in the interval $[-1, +\infty[$. For any feasible $\bar{x} \in [-1, +\infty[$, the set of lower-level optimal solutions is given by:

$$\phi(\bar{x}) = \left\{ (y_1, y_2) \in \mathbb{R}^2 : y_1 + y_2 = 1 + \bar{x};\ y_1, y_2 \geq 0 \right\}.$$

Given the upper-level objective, we can compute the optimistic y^O and pessimistic y^P solutions as:

$$\begin{aligned} y^O &= (y_1^O, y_2^O) = (0, 1 + \bar{x}) \\ y^P &= (y_1^P, y_2^P) = (1 + \bar{x}, 0). \end{aligned}$$

By replacing these lower-level solutions into the upper-level objective, we obtain $-2x - 1$ in the optimistic version, and 1 in the pessimistic formulation. Consequently, for the optimistic formulation, we can build a direction of unboundedness $(\Delta x, \Delta y_1, \Delta y_1) = (1, 0, 1)$ valid for the feasible point $(x, y_1, y_2) = (-1, 0, 0)$.

Therefore, the optimistic formulation of the bilevel problem is unbounded. However, the pessimistic formulation has a constant upper-level objective value for all feasible solutions. Therefore, the pessimistic formulation of the bilevel problem is bounded. In conclusion, unboundedness of the optimistic formulation of a bilevel problem does not imply that of its pessimistic formulation.

C Checking Unboundedness in Multilevel Optimization

In this section, we prove Theorem 3 showing that Unbounded-KLP is strongly Σ^p_{k-1}-hard. We have divided the proof into smaller proofs showing that checking unboundedness of a linear trilevel model and a k-level problem for $k \geq 4$ are Σ^p_2-hard and Σ^p_{k-1}-hard, respectively. We have further divided the proof for the k-level problem into cases where k is odd and even. The decision problem that we use in all these smaller proofs is the $(k-1)$-Alternating Quantified Satisfiability with k adjusted as suited:

$(k-1)$-Alternating Quantified Satisfiability:
INSTANCE: Disjoint non-empty sets of variables $X_1, \ldots, X_{k-1}$, a boolean expression E over $\bigcup_{l=1}^{k-1} X_l$ in a conjunctive normal form with at most 3 literals in each clause $c \in C$.
QUESTION:

- When k odd, $(\mathcal{B}_{k-1} \cap \overline{\text{3CNF}})$: Is there a truth assignment a_{k-1} of the variables in X_{k-1} such that for all truth assignments a_{k-2} of the variables in X_{k-2}, ..., such that for all truth assignments a_1 of the variables in X_1 the expression E is not satisfied?
- When k even, $(\mathcal{B}_{k-1} \cup \text{3CNF})$: Is there a truth assignment a_{k-1} of the variables in X_{k-1} such that for all truth assignments a_{k-2} of the variables in X_{k-2}, ..., such that there is a truth assignment a_1 of the variables in X_1 such that the expression E is satisfied?

C.1 Trilevel Unboundedness Problem is Σ_2^p-hard

Based on the 2-Alternating Quantified Satisfiability $(\mathcal{B}_2 \cap \overline{\text{3CNF}})$ problem, we show that deciding whether a linear trilevel problem is unbounded is a Σ_2^p-hard problem in Theorem 6.

Theorem 6. Unbounded-KLP *for $k = 3$ is Σ_2^p-hard.*

Proof. Let $k = 3$. We show that an instance of Unbounded-KLP reduces to an instance of $\mathcal{B}_2 \cap \overline{\text{3CNF}}$. Given as instance of $\mathcal{B}_2 \cap \overline{\text{3CNF}}$, we build the following Unbounded-KLP instance:

$$
\begin{aligned}
\max_{\substack{y, x_2,\\ x_1, z_1, z_2}} \quad & \sum_{i=1}^{n_1} (z_1)_i \\
\text{s.t.} \quad & y \geq 1 \\
& 0 \leq x_2 \leq y \\
& z_2 = 0 \\
& (x_1, z_1, z_2) \in \arg\min_{x_1, z_1, z_2} \quad \sum_{i=1}^{n_1} (z_1)_i \\
& \qquad \text{s.t.} \quad 0 \leq x_1 \leq y \\
& \qquad\qquad \sum_{i=1}^{2} A_i x_i \geq (1+b) y \\
& \qquad\qquad (z_1, z_2) \in \arg\max_{z_1, z_2} \quad \sum_{i=1}^{n_1} (z_1)_i + \sum_{i=1}^{n_2} (z_2)_i \\
& \qquad\qquad\qquad \text{s.t.} \quad z_1 \leq x_1 \\
& \qquad\qquad\qquad\qquad z_1 \leq y - x_1 \\
& \qquad\qquad\qquad\qquad z_2 \leq x_2 \\
& \qquad\qquad\qquad\qquad z_2 \leq y - x_2.
\end{aligned}
\tag{3LP}
$$

Note that the only linking constraint is $z_2 = 0$ at level 3 which enforces that $x_2 \in \{0, y\}$. In addition, optimality of level 1 implies that at any feasible solution we have that $(z_1)_i = \min\{(x_1)_i, y - (x_1)_i\}$ $\forall i \in \{1, \dots, n_1\}$ and $(z_2)_i = \min\{(x_2)_i, y - (x_2)_i\}$ $\forall i \in \{1, \dots, n_2\}$. Optimality of level 2 implies that given (y, x_2), if a 'discrete' $x_1 \in \{0, y\}^{n_1}$ exists, it will be selected over any feasible x_1 where $\exists i : (x_1)_i \in]0, y[$.

We show that $\mathcal{B}_2 \cap \overline{\text{3CNF}}$ is a YES instance if and only if (3LP) is unbounded.

Proof of if. Assume that $\mathcal{B}_2 \cap \overline{\text{3CNF}}$ is a YES instance, this is that $\exists a_2 \in \{0,1\},\ \forall a_1 \in \{0,1\} : A_1 a_1 + A_2 a_2 < 1 + b$. Equivalently, we can write:

$$\exists a_2 \in \{0,1\},\ \forall a_1 \in [0,1] : A_1 a_1 + A_2 a_2 \geq 1 + b \Rightarrow \exists i : (a_1)_i \in]0,1[.$$

Let $x_2 = a_2$, $y = 1$, $z_2 = \min\{(a_2)_i, 1 - (a_2)_i\} = 0$. Pick $x_1 \in [0, y]$ such that $A_1 x_1 + A_2 a_2 \geq (1 + b) y$ and that minimizes the sum of 'discrete' violations $\sum_{i=1}^{n_1} (z_1)_i = \sum_{i=1}^{n_1} \min\{(x_1)_i, y - (x_1)_i\}$. By assumption, we have that $\exists j : (x_1)_j \in]0, y[$. Consequently, we know that $(z_1)_j > 0$. This solution is feasible for (3LP), because it verifies all constraints as well as optimality of level 1 and 2.

Moreover, $\Delta y = 1$, $\Delta x_2 = \Delta y x_2$, $\Delta z_2 = 0$, $\Delta x_1 = \Delta y x_1$, $\Delta z_1 = \Delta y z_1$ is a direction of unboundedness for (3LP). It is possible to verify that $(y, x_2, x_1, z_2, z_1) + k(\Delta y, \Delta x_2, \Delta x_1, \Delta z_2, \Delta z_1)$ is a feasible point for any $k \geq 0$, and we also have that $\sum_{i=1}^{n_1} (\Delta z_1)_i \geq (z_1)_j > 0$. Therefore, the trilevel problem (3LP) is unbounded.

Proof of only if. Assume that $\mathcal{B}_2 \cap \overline{\text{3CNF}}$ is a NO instance, this is that $\neg(\exists a_2 \in \{0,1\},\ \forall a_1 \in \{0,1\} : A_1 a_1 + A_2 a_2 < 1 + b)$. Equivalently, we can write:

$$\forall a_2 \in \{0,1\},\ \exists a_1 \in [0,1] : A_1 a_1 + A_2 a_2 \geq 1 + b.$$

This implies that for all $x_2 \in [0, y]$ such that $z_2 = 0$, this is $x_2 \in \{0, y\}$, there exists $x_1 \in \{0, y\}^{n_1}$ such that $A_1 x_1 + A_2 a_2 \geq (1 + b) y$. Note that the objective of level 2 is to minimise $\sum_{i=1}^{n_1} (z_1)_i$ which is minimised at 0 when $x_1 \in \{0, y\}$. Consequently, for any x_2 selected, optimality of level 2 will imply that $x_1 \in \{0, y\}$ (which we know exists by assumption).

In turn, this implies that any feasible solution (y, x_2, x_1, z_2, z_1) has $z_1 = 0$. Consequently, the objective of level 3 is bounded above by 0 ($\sum_{i=1}^{n_1} (z_1)_i \leq 0$). Therefore, the 3-level problem (3LP) is not unbounded. □

C.2 Unbounded-KLP with Odd k is Σ_{k-1}^p-hard

Throughout this section, we assume $k \geq 4$ is an odd number. Based on the $(k-1)$-Alternating Quantified Satisfiability ($\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$) problem, we show that Unbounded-KLP where k is odd is a Σ_{k-1}^p-hard problem in Theorem 7.

Theorem 7. Unbounded-KLP *for k odd is Σ_{k-1}^p-hard.*

Proof. We show that an instance of UNBOUNDED-KLP reduces to an instance of $\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$. Given as instance of $\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$, we build the following UNBOUNDED-KLP instance:

$$\begin{array}{rll}
\max\limits_{y,x,z} & \sum\limits_{i=1}^{n_1} (z_1)_i & \\
\text{s.t.} & y \geq 1 & \\
& 0 \leq x_{k-1} \leq y & \\
& z_l = 0 \quad \forall l \geq 2 & \\
& \vdots & \\
l \text{ odd:} & (x^{(l)}, z) \in \arg\min\limits_{x^{(l)},z} & \left\{ \sum\limits_{i=1}^{n_1} (z_1)_i : 0 \leq x_l \leq y;\ (x^{(l-1)}, z) \in \Phi^{l-1} \right\} \\
l \text{ even:} & (x^{(l)}, z) \in \arg\max\limits_{x^{(l)},z} & \left\{ \sum\limits_{i=1}^{n_1} (z_1)_i : 0 \leq x_l \leq y;\ (x^{(l-1)}, z) \in \Phi^{l-1} \right\} \\
& \vdots & \\
& (x_1, z) \in \arg\min\limits_{x_1,z} & \sum\limits_{i=1}^{n_1} (z_1)_i \\
& \qquad\qquad \text{s.t.} & 0 \leq x_1 \leq y \\
& & \sum\limits_{i=1}^{k-1} A_i x_i \geq (1+b) y \\
& & (z) \in \arg\max\limits_{z} \ \sum\limits_{l=1}^{k-1} \sum\limits_{i=1}^{n_l} (z_l)_i \\
& & \qquad\quad \text{s.t.} \ (z_l)_i \leq (x_l)_i \qquad \forall l,\ \forall i \\
& & \qquad\qquad\ \ (z_l)_i \leq y - (x_l)_i \quad \forall l,\ \forall i
\end{array} \tag{Odd-KLP}$$

where $z = (z_1, \ldots, z_{k-1})$, $x^{(i)} = (x_1, \ldots, x_i)$, $x = (x_1, \ldots, x_{k-1})$, and Φ^i is the problem at level i parameterised by the variables $(y, x_{k-1}, \ldots, x_{i+1})$ of the levels above.

Note that the only linking constraints are $z_l = 0\ \forall l \in \{2, \ldots, k-1\}$ at level k which enforces that for $l \in \{2, \ldots, k-1\} : x_l \in \{0, y\}^{n_l}$. In addition, optimality of level 1 implies that at any feasible solution we have that $(z_l)_i = \min\{(x_l)_i, y - (x_l)_i\}\ \forall i \in \{1, \ldots, n_l\}, \forall i \in \{1, \ldots, n_1\}$. Optimality of level 2 implies that given $(y, x_{k-1}, ..., x_2)$, if a feasible 'integer' $x_1 \in \{0, y\}^{n_1}$ exists, it will be selected over any feasible x_1 where $\exists i : (x_1)_i \in]0, y[$.

We show that $\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$ is a YES instance if and only if (Odd-KLP) is unbounded.

Proof of if. Assume that $\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$ is a YES instance, this is that $\exists a_{k-1} \in \{0,1\}^{n_{k-1}},\ \ldots,\ \exists a_2 \in \{0,1\}^{n_2},\ \forall a_1 \in \{0,1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l < 1 + b$. Equivalently, we can write $\exists a_{k-1} \in \{0,1\}^{n_{k-1}},\ \ldots,\ \exists a_2 \in \{0,1\}^{n_2}$ such that

$$\forall a_1 \in [0,1]^{n_1} : \sum_{l=1}^{k-1} A_l a_l \geq 1 + b \Rightarrow \exists j : (a_1)_j \in]0, 1[.$$

Let $l \in \{3, \ldots, k-1\}$.

1. When l is odd:

   Given a feasible $(y, x_{k-1}, \dots, x_l)$, then we know by assumption that $\exists x_{l-1} \in \{0, y\}^{n_{l-1}},\ \dots,\ \exists x_2 \in \{0, y\}^{n_2}$ such that

   $$\forall x_1 \in [0, y]^{n_1} : \sum_{l=1}^{k-1} A_l x_l \geq (1 + b)y \Rightarrow \exists j : (x_1)_j \in]0, y[.$$

   Since a solution where $x_1 \notin \{0, y\}$ results in a strictly positive value for $\sum_{i=1}^{n_1} (z_1)_i > 0$ at level l whose goal is to maximize this sum, then an x_{l-1} that results in $\sum_{i=1}^{n_1} (z_1)_i > 0$ will always be selected.

2. When l is even:

   Given a feasible $(y, x_{k-1}, \dots, x_l)$, then we know by assumption that $\forall x_{l-1} \in \{0, y\}^{n_{l-1}},\ \dots,\ \exists x_2 \in \{0, y\}^{n_2}$ such that

   $$\forall x_1 \in [0, y]^{n_1} : \sum_{l=1}^{k-1} A_l x_l \geq (1 + b)y \Rightarrow \exists j : (x_1)_j \in]0, y[.$$

   Therefore, any solution to level i will have strictly positive objective value (as $\sum_{i=1}^{n_1} (z_1)_i \geq (z_1)_j > 0$).

Note that, when $l \leq k - 2$, the problem at level l is not unbounded because y is a decision of level $k - 1$ and hence a parameter for this level.

Nevertheless, the fact that an optimal solution of level l has a strictly positive objective value $\sum_{i=1}^{n_1} (z_1)_i > 0$ allows us to build a direction of unboundedness for the k-level problem as:

$$\begin{aligned}
&\Delta y \ = 1 \\
&\Delta z_2 = \cdots = \Delta z_{k-1} = 0 \\
&\Delta z_1 = \Delta y \cdot z_1 \\
&\Delta x_l = \Delta y \cdot x_l \quad \forall l \{1, \dots, k - 1\}
\end{aligned}$$

where $y = 1$, $x_l = a_l\ \forall l \in \{2, \dots, k - 1\}$, $(z_1)_i = \min\{(a_1)_i, 1 - (a_1)_i\}\ \forall i \in \{1, \dots, n_1\}$ and $z_2 = 0\ \forall l \in \{2, \dots, k - 1\}$ is a feasible solution. So, at each odd level l, a_l is selected to maximise $\sum_{i=1}^{n_1} (z_1)_i$ and at each even level l, a_l is selected to maximise $\sum_{i=1}^{n_1} (z_1)_i$. Therefore, (Odd-KLP) is unbounded.

Proof of only if. Assume that $\mathcal{B}_{k-1} \cap \overline{\text{3CNF}}$ is a NO instance, this is that $\neg(\exists a_{k-1} \in \{0, 1\}^{n_{k-1}},\ \dots,\ \exists a_2 \in \{0, 1\}^{n_2},\ \forall a_1 \in \{0, 1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l < 1 + b)$. Equivalently, we can write:

$$\forall a_{k-1} \in \{0, 1\}^{n_{k-1}},\ \dots,\ \forall a_2 \in \{0, 1\}^{n_2},\ \exists a_1 \in \{0, 1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l \geq 1 + b.$$

Let $l \in \{3, \dots, k - 1\}$.

1. When l is odd:

   Given a feasible $(y, x_{k-1}, \ldots, x_l)$, then we know by assumption that $\forall x_{l-1} \in \{0, y\}^{n_{l-1}},\ \ldots,\ \forall x_2 \in \{0, y\}^{n_2},\ \exists x_1 \in \{0, y\}^{n_1} : \sum_{l=1}^{k-1} A_l x_l \geq (1 + b)y$.

   Therefore, any feasible solution x_{l-1} selected at level l results in an 'integer' $x_1 \in \{0, y\}$ and consequently an objective value of $\sum_{i=1}^{n_1} (z_1)_i = 0$.

2. When l is even:

   Given a feasible $(y, x_{k-1}, \ldots, x_l)$, then we know by assumption that $\exists x_{l-1} \in \{0, y\}^{n_{l-1}},\ \ldots,\ \forall x_2 \in \{0, y\}^{n_2},\ \exists x_1 \in \{0, y\}^{n_1} : \sum_{l=1}^{k-1} A_l x_l \geq (1 + b)y$.

   Given that such a decision x_{l-1} would result in an 'integer' $x_1 \in \{0, y\}^{n_1}$ and hence minimise the objective function $\sum_{i=1}^{n_1} (z_1)_i$ at 0, then that would be the optimal solution of level l.

We conclude that any feasible solution of the (Odd-KLP) model has objective value $\sum_{i=1}^{n_1} (z_1)_i$ bounded above by 0. Therefore, (Odd-KLP) is not unbounded. □

C.3 Unbounded-KLP with Even k is Σ_{k-1}^p-hard

Throughout this section, we assume $k \geq 4$ is an even number. Based on the $(k-1)$-ALTERNATING QUANTIFIED SATISFIABILITY ($\mathcal{B}_{k-1} \cup$3CNF) problem, we show UNBOUNDED-KLP where k is even is a Σ_{k-1}^p-hard problem in Theorem 8.

Theorem 8. UNBOUNDED-KLP *for k even is Σ_{k-1}^p-hard.*

Proof. We show that an instance of UNBOUNDED-KLP reduces to an instance of $\mathcal{B}_{k-1} \cup$ 3CNF. Given as instance of $\mathcal{B}_{k-1} \cup$ 3CNF, we build the following

Unbounded-KLP instance:

$$
\begin{array}{rll}
\max\limits_{y,x,z} & y & \\
\text{s.t.} & y \geq 1 & \\
& 0 \leq x_{k-1} \leq y & \\
& z_l = 0 \quad \forall l \geq 1 & \\
& \vdots & \\
l \text{ even:} & (x^{(l)}, z) \in \arg\max\limits_{x^{(l)},z} & \left\{ \sum\limits_{i=1}^{n_1} (z_1)_i : 0 \leq x_l \leq y;\ (x^{(l-1)}, z) \in \Phi^{l-1} \right\} \\
l \text{ odd:} & (x^{(l)}, z) \in \arg\min\limits_{x^{(l)},z} & \left\{ \sum\limits_{i=1}^{n_1} (z_1)_i : 0 \leq x_l \leq y;\ (x^{(l-1)}, z) \in \Phi^{l-1} \right\} \\
& \vdots & \\
& (x_1, z) \in \arg\min\limits_{x_1,z} & \sum\limits_{i=1}^{n_1} (z_1)_i \\
& \text{s.t.} & 0 \leq x_1 \leq y \\
& & \sum\limits_{i=1}^{k-1} A_i x_i \geq (1+b)y \\
& & (z) \in \arg\max\limits_{z} \sum\limits_{l=1}^{k-1} \sum\limits_{i=1}^{n_l} (z_l)_i \\
& & \qquad \text{s.t.} \quad (z_l)_i \leq (x_l)_i \qquad \forall l,\ \forall i \\
& & \qquad \qquad (z_l)_i \leq y - (x_l)_i \quad \forall l,\ \forall i
\end{array}
\tag{Even-KLP}
$$

where $z = (z_1, \ldots, z_{k-1})$, $x^{(i)} = (x_1, \ldots, x_i)$, $x = (x_1, \ldots, x_{k-1})$, and Φ^i is the problem at level i parameterised by the variables $(y, x_{k-1}, \ldots, x_{i+1})$ of the levels above.

Note that the only linking constraints are $z_l = 0\ \forall l \in \{1, \ldots, k-1\}$ at level k. In addition, optimality of level 1 implies that at any feasible solution we have that $(z_l)_i = \min\{(x_l)_i, y - (x_l)_i\}\ \forall i \in \{1, \ldots, n_l\}, \forall l \in \{1, \ldots, k-1\}$. This together with the linking constraints enforces that for $l \in \{1, \ldots, k-1\} : x_l \in \{0, y\}^{n_l}$. Optimality of level 2 implies that given $(y, x_{k-1}, ..., x_2)$, if a feasible 'integer' $x_1 \in \{0, y\}^{n_1}$ exists, it will be selected over any feasible x_1 where $\exists i : (x_1)_i \in]0, y[$.

We show that $\mathcal{B}_{k-1} \cup$ 3CNF is a YES instance if and only if (Even-KLP) is unbounded.

Proof of if. Assume that $\mathcal{B}_{k-1} \cup$3CNF is a YES instance, this is that $\exists a_{k-1} \in \{0,1\}^{n_{k-1}}$, $\forall a_{k-2} \in \{0,1\}^{n_{k-2}}$, $\ldots$, $\forall a_2 \in \{0,1\}^{n_2}$, $\exists a_1 \in \{0,1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l \geq 1 + b$.

Let $x_{k-1} = a_{k-1}$ be one such assignment, and $y = 1$.

For odd $l \in \{k-3, k-5, \ldots, 3\}$, the corresponding level whose goal is to minimize $\sum_{i=1}^{n_l} (z_l)_i$ will choose $x_{l-1} = a_{l-1}$ as the assignment that results in $x_1 = a_1 = 0$ at the second level, which we know exists for whatever decision the level above $l+1$ took. For even $l \in \{k-2, k-4, \ldots, 2\}$, no matter which decision is taken, we know results in an objective value of 0, because the level that follows $l+1$ (is odd) will choose $x_l = a_l$ in order to enforce $x_1 \in \{0, y\}$. A solution build this way and with $y = 1$ and $z_l = 0\ \forall l \in \{1, \ldots, k-1\}$ is feasible for the model (Even-KLP), and has objective value 1.

Furthermore, $\Delta y = 1$, $\Delta z_l = 0$ and $\Delta x_l = \Delta y \cdot a_l$ for $l \in \{1, \ldots, k-1\}$ is a direction of unboundedness for the model (Even-KLP). Namely, $\Delta y = 1 > 0$. Therefore, the model (Even-KLP) is unbounded.

Proof of only if. Assume that $\mathcal{B}_{k-1} \cup 3\text{CNF}$ is a NO instance, this is that $\forall a_{k-1} \in \{0,1\}^{n_{k-1}}$, $\exists a_{k-2} \in \{0,1\}^{n_{k-2}}$, $\ldots$, $\exists a_2 \in \{0,1\}^{n_2}$, $\forall a_1 \in [0,1]^{n_1}$ such that:

$$\sum_{l=1}^{k-1} A_l a_l \geq 1 + b \Rightarrow \exists j : (x_1)_j \in]0,1[.$$

This implies that no matter which assignment the x_l the odd levels $l \in \{k-1, k-3, \ldots, 3\}$ select, then even level will select $x_{k-2}, \ldots, x_2$, which we know exist by assumption, that result in a 'non-integer' assignment a_1 at level 2. Consequently, no matter which assignment x_{k-1} is chosen at level k, we know there exists j such that $(x_1)_j \in]0, y[$. Consequently, $(z_1)_j > 0$ and the linking constraint $z_1 = 0$ is violated.

Therefore, there is no feasible solution to the model (Even-KLP). Hence, this model is NOT unbounded. □

D LPCC Reformulation Result

In this appendix, we present the detailed proof of Theorem 4, which states that the bilevel problem (B) is unbounded if and only if the linear complementarity problem (U) has strictly negative optimal value.

Proof. According to Lemma 1 and Theorem 1, we can prove this theorem by showing the following equivalence instead: There exists $\omega \in \{1,2\}^{n_2}$ such that (P_ω) is unbounded if and only if (U) has strictly negative optimal value.

Proof of if. Assume that there exists $\omega \in \{1,2\}^{n_2}$ such that the linear problem (P_ω) is unbounded. Then, we know that there exists a feasible point $(x^\star, y^\star, \lambda^\star) \in \mathcal{P}_\omega$ and a corresponding direction of unboundedness $(\Delta x^\star, \Delta y^\star, \Delta\lambda^\star)$. Without loss of generality, we assume that this direction is normalised ($\|\Delta x^\star, \Delta y^\star, \Delta\lambda^\star\| = 1$) such that constraint (U.7) holds. Note that, since there is the bilevel feasible solution $(x^\star, y^\star, \lambda^\star)$, we know that problem (U) is finite optimal (because $(x^\star, y^\star, \lambda^\star, 0, 0)$ is a feasible solution and constraint (U.7) ensures boundedness).

We now show that there is a feasible solution for (U) with negative objective value. Since $(x^\star, y^\star, \lambda^\star) \in \mathcal{P}_\omega$, then $(x^\star, y^\star, \lambda^\star)$ verifies constraints (U.2)-(U.3). Furthermore since $(\Delta x^\star, \Delta y^\star, \Delta\lambda^\star)$ is a direction of unboundedness for (P_ω) and $(x^\star, y^\star, \lambda^\star) \in \mathcal{P}_\omega$, then we know that $(\Delta x^\star, \Delta y^\star, \lambda^\star)$ verifies constraints (U.4)-(U.6). Therefore, $(x^\star, y^\star, \lambda^\star, \Delta x^\star, \Delta y^\star)$ is a feasible solution of problem (U). Moreover, since $(\Delta x^\star, \Delta y^\star, \Delta\lambda^\star)$ is a direction of unboundedness for (P_ω), we have that $c^\top \Delta x^\star + d^\top \Delta y^\star < 0$. Consequently, we can conclude that problem (U) has strictly negative objective value.

Proof of only if. Assume that the problem (U) has strictly negative optimal objective value and $(x^\star, y^\star, \lambda^\star, \Delta x^\star, \Delta y^\star)$ is one of its optimal solutions. Then, we define $\omega^\star$ such that $\omega^\star_i = 1$ when $\lambda^\star_i > 0$ and $\omega^\star_i = 2$ when $\lambda^\star_i = 0$. From constraints (U.2)-(U.3), the point $(x^\star, y^\star, \lambda^\star)$ is feasible for problem (P_ω). Furthermore, from constraints (U.4)-(U.6), we can ensure that along the direction $(\Delta x^\star, \Delta y^\star, \vec{0})$ there is a sequence $\{(x^\star, y^\star, \lambda^\star) + k(\Delta x^\star, \Delta y^\star, \vec{0})\}_{k\in\mathbb{Z}_0^+}$ of feasible points for problem (P_ω). Finally, from the fact that the optimal objective value is strictly negative, we know that as k increases, the objective value of (P_ω) at the points in this sequence decreases. Hence, there exists $\omega \in \{1,2\}^{n_2}$ (as defined from the optimal values of $\lambda^\star$) such that the linear problem (P_ω) is unbounded.

□

E Auxiliary Results for Lemma 2

In this section, we prove Lemma 4 which we have used to obtain Lemma 2.

Lemma 4. *Let $\omega \in \{1,2\}^{n_2}$. If $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a vertex of $\mathcal{P}_\omega$, then $(\tilde{x}, \tilde{y})$ is a vertex of the HPR's feasible set.*

Proof. We show this result by showing two implications:

a) If $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a vertex of $\mathcal{P}_\omega$, then $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a vertex of the feasible set $\mathcal{F}$.

b) If $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a vertex of $\mathcal{F}$, then $(\tilde{x}, \tilde{y})$ is a vertex of the HPR's feasible set.

Proof of implication a) Note that, since $\mathcal{P}_\omega$ is a restriction of $\mathcal{F}$ where some inequalities are enforced as equalities, the set of constraint coefficients $\{M_i\}_{i\in\{1,\dots,n\}}$ is the same for both polyhedra, where $n = n_1 + n_2 + 2n_y$ is the number of constraints. For illustration, the coefficients M_i are defined as $M_i = [A_i \; B_i \; \vec{0}]$ for $i \in \{1,\dots,n_1\}$, $M_i = [C_{i-n_1} \; D_{i-n_1} \; \vec{0}]$ for $i \in \{n_1 + 1,\dots,n_1+n_2\}$, $M_i = [\vec{0} \; \vec{0} \; D^\top_{i-n_1-n_2}]$ for $i \in \{n_1+n_2+1,\dots,n_1+n_2+n_y\}$, and $M_i = [\vec{0} \; \vec{0} \; e^\top_{i-n_1-n_2-n_y}]$ for $i \in \{n_1+n_2+n_y,\dots,n_1+n_2+2n_y\}$ where e_i is the i^{th} unit vector. The same holds true for the right-hand-side coefficients $\{r_i\}_{i\in\{1,\dots,n\}}$ of both polyhedra.

Let $\omega \in \{1,2\}^{n_2}$, and $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ a vertex of $\mathcal{P}_\omega$. Then $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a basic feasible solution of $\mathcal{P}_\omega$ which means that $(\tilde{x}, \tilde{y}, \tilde{\lambda}) \in \mathcal{P}_\omega$, and that the set of coefficients of the active constraints at $(\tilde{x}, \tilde{y}, \tilde{\lambda})$,

$$I(\tilde{x}, \tilde{y}, \tilde{\lambda}) = \Big\{ M_i : M_i(\tilde{x}, \tilde{y}, \tilde{\lambda}) = r_i \;\forall i \in \{1,\dots,n\} \Big\}$$

contains $n_x+n_y+n_\lambda$ linearly independent vectors, where $n_x+n_y+n_\lambda$ represents the number of decision variables (x, y, λ).

Since $\mathcal{P}_\omega \subseteq \mathcal{F}$, then $(\tilde{x}, \tilde{y}, \tilde{\lambda}) \in \mathcal{F}$ is a feasible solution. Moreover, since the constraint coefficients M_i and right-hand-side coefficients r_i are the same for both $\mathcal{P}_\omega$ and $\mathcal{F}$ and since $I(\tilde{x}, \tilde{y}, \tilde{\lambda})$ contains $n_x+n_y+n_\lambda$ linearly independent vectors, then $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a basic solution of $\mathcal{F}$. Thus, $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a basic feasible solution of $\mathcal{F}$, that is $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ is a vertex of $\mathcal{F}$.

Proof of implication b) Let $(\tilde{x}, \tilde{y}, \tilde{\lambda})$ a vertex of $\mathcal{F}$. Then, there exists a supporting hyperplane of $\mathcal{F}$: $\mathcal{H} = \{(x, y, \lambda) : a_x^\top x + a_y^\top y + a_\lambda^\top \lambda = \alpha\}$ such that

$$\mathcal{F} \cap \mathcal{H} = \{(\tilde{x}, \tilde{y}, \tilde{\lambda})\}$$
$$\mathcal{F} \subseteq \mathcal{H}^+ = \{(x, y, \lambda) : a_x^\top x + a_y^\top y + a_\lambda^\top \lambda \geq \alpha\}.$$

We show that $(\tilde{x}, \tilde{y})$ is a vertex of the HPR's feasible set ($\mathcal{F}_{\text{HPR}}$) by showing that $\hat{\mathcal{H}} = \{(x, y) : a_x^\top x + a_y^\top y = \beta\}$ where $\beta = \alpha - a_\lambda^\top \tilde{\lambda}$ is a supporting hyperplane of the HPR's feasible set which intersects it at $(\tilde{x}, \tilde{y})$.

First, we want to show that $\mathcal{F}_{\text{HPR}} \cap \hat{\mathcal{H}} = \{(\tilde{x}, \tilde{y})\}$. Assume, by contradiction, that there exists $(x', y') \neq (\tilde{x}, \tilde{y})$ such that $(x', y') \in \mathcal{F}_{\text{HPR}} \cap \hat{\mathcal{H}}$. By the definition of $\hat{\mathcal{H}}$, we have that $(x', y', \tilde{\lambda}) \in \mathcal{H}$. And since $(x', y') \in \mathcal{F}_{\text{HPR}}$, we also know that $(x', y', \tilde{\lambda}) \in \mathcal{F}$. Therefore, $(x', y', \tilde{\lambda}) \in \mathcal{F} \cap \mathcal{H}$, which is a contradiction because $(x', y', \tilde{\lambda}) \neq (\tilde{x}, \tilde{y}, \tilde{\lambda})$ and $\mathcal{F} \cap \mathcal{H} = \{(\tilde{x}, \tilde{y}, \tilde{\lambda})\}$. Hence, $\mathcal{F}_{\text{HPR}} \cap \hat{\mathcal{H}} = \{(\tilde{x}, \tilde{y})\}$.

Second, we want to show that $\mathcal{F}_{\text{HPR}} \subseteq \hat{\mathcal{H}}^+ = \{(\tilde{x}, \tilde{y}) : a_x^\top x + a_y^\top y \geq \alpha\}$. Let $(x, y) \in \mathcal{F}_{\text{HPR}}$. Then, we have that $(x, y, \tilde{\lambda}) \in \mathcal{F}$ and that $\mathcal{F} \subseteq \mathcal{H}^+$. Thus, $(x, y, \tilde{\lambda}) \in \mathcal{H}^+$. Given the definitions of $\mathcal{H}^+$ and $\hat{\mathcal{H}}^+$, we conclude that $(x, y) \in \hat{\mathcal{H}}^+$. Hence, $\mathcal{F}_{\text{HPR}} \subseteq \hat{\mathcal{H}}^+$.

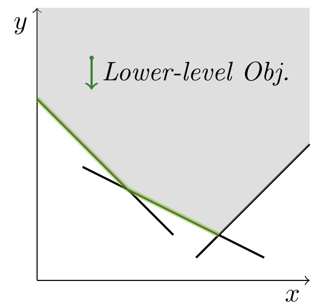
Finally, since $\hat{\mathcal{H}}$ is a supporting hyperplane of $\mathcal{F}_{\text{HPR}}$ which intersects it at $(\tilde{x}, \tilde{y})$, then $(\tilde{x}, \tilde{y})$ is a vertex of $\mathcal{F}_{\text{HPR}}$.

□

F Insights from Example of Bounded Bilevel Problem with Unbounded HPR

Example 3 (Bounded Bilevel)**.** *Consider the unbounded bilevel model below and the corresponding graph, where the bilevel feasible region is colored green, and the direction is that of improving lower-level objective.*

$$\begin{aligned} \min_{x\geq 0, y} \quad & -x-y \\ s.t. \quad & x-y \leq 3 \\ & y \in \arg\min_{\tilde{y}\geq 0}\{\tilde{y} : \quad -x-2\tilde{y} \leq -6 \\ & \qquad\qquad\qquad\quad -x-\tilde{y} \leq -4\}, \end{aligned}$$



In this example, the HPR is unbounded along the direction $(\Delta x, \Delta y) = (1, 1)$. *However, the bilevel feasible region (in green) is bounded, and the bilevel problem is finite optimal with optimal solution* $(x, y) = (4, 1)$.

Confirming this boundedness of the bilevel problem, the LPCC (U) has optimal value 0, and the vertex-enumeration Algorithm 1 does not find any direction of unboundedness of the bilevel.

In our implementation, the vertex-enumeration algorithm enumerates all possible basis to get to this conclusion. For example, when it finds the basic feasible solution associated with the vertex $(x, y) = (4, 1)$, *where the basic variables are* x, y *and the slack of the second lower-level constraint, it detects unboundedness of the HPR. In fact, in its simplex tableaux, the non-basic slack variable of the first lower-level constraint has a negative reduced cost of* $\bar{c}_i = -\frac{2}{3}$, *and a non-positive nonzero column is* $\bar{A}_{\cdot,i} = [-\frac{1}{3} \;\; -\frac{1}{3} \;\; -\frac{2}{3}]^\top$. *Therefore, following step 6, we build a direction of unboundedness for the HPR as* $(\Delta x, \Delta y) = (\frac{1}{3}, \frac{1}{3})$ *(and* $(0, 1, \frac{2}{3})$ *for the three slack variables). In this case the model (U') is infeasible. From constraints (U.6), we have that both dual variables,* λ_1 *and* λ_2, *are forced to* 0. *However, the dual constraint states that* $-2\lambda_1 - \lambda_2 = -1$. *These simultaneous restrictions on* λ_1 *and* λ_2 *deem the problem (U') infeasible. Thus, Algorithm 1 discards this basis, and keeps searching. As a matter of fact, since the bilevel is bounded, all bases are discarded either because (a) they do not yield a basic feasible solution of the HPR, (b) they do not yield a bilevel feasible solution, (c) there is no direction of unboundedness of the HPR at the solution, (d) there are no feasible dual values from (U') at the point and direction obtained.*