Unboundedness in Bilevel Optimization

Bárbara Rodrigues[1*], Margarida Carvalho[2], Miguel F. Anjos[1,3], Nagisa Sugishita[2]

[1*]School of Mathematics and Maxwell Institute for Mathematical Sciences, University of Edinburgh, Edinburgh, EH9 3FD, Midlothian, United Kingdom.

[2]CIRRELT and Département d'informatique et de recherche opérationnelle, Université de Montréal, Montreal, H3T 1J4, Quebec, Canada.

[3]GERAD, Polytechnique Montréal, Montreal, H3T 2A7, Quebec, Canada.

*Corresponding author(s). E-mail(s): B.C.Rodrigues@sms.ed.ac.uk; Contributing authors: carvalho@iro.umontreal.ca; anjos@stanfordalumni.org; nagisa.sugishita@umontreal.ca;

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 and multilevel optimization by studying its computational complexity. We show that deciding whether an optimistic linear bilevel problem is unbounded is strongly NP-complete, even without linking constraints. Furthermore, we extend the hardness result to the linear multilevel case, by showing that for each extra level added, the decision problem of checking unboundedness moves up a level in the polynomial hierarchy. Deciding unboundedness of a mixed-integer multilevel problem is shown to be one level higher in the polynomial complexity hierarchy than the decision problem for linear multilevel problem with the same number of levels. 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 proof of concept of these algorithmic approaches on some relevant examples, and provide a brief computational comparison.

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 [1, 2] 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 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 [3].

Bilevel problems are known to be challenging to solve. For instance, mixed-integer bilevel problems are shown to be Σ_2^p-hard in [4]. In fact, even in their simplest form with linear objective functions and constraints, bilevel problems are strongly NP-hard [5]. In this paper, we focus on this linear case of bilevel problems, whose optimistic formulation is expressed in (B):

$$
\begin{aligned}
\min_{x,y} \quad & c^\top x + d^\top y && \text{(B.1)}\\
\text{s.t.} \quad & Ax + By \le a, && \text{(B.2)}\\
& y \in \arg\min_{\tilde{y}} \quad f^\top \tilde{y} && \text{(B.3)}\\
& \qquad\quad \text{s.t.} \quad Cx + D\tilde{y} \le b, && \text{(B.4)}
\end{aligned}
$$

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. [6] showed in 1997 that a binary variable $x \in \{0,1\}$ can be modelled by the constraints $y = 0$, $0 \le x \le 1$, and the linear continuous problem:

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

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 [7], and it might even be disconnected [8, 9] in the presence of linking constraints (also known as coupling constraints), this is if $B \neq \mathbf{0}$.

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 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 problem exists, it can be found at a vertex of this relaxation's feasible set [7], 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 problem. The examples in [10] show that when the HPR model is unbounded, the corresponding bilevel model 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 [11–14]. Consequently, there is little existing research on how to handle bilevel problems when this relaxation is unbounded.

1.1 Motivation

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 [15, 16]. This key lemma has driven most of the results in this field. Note that this result is derived for mixed-integer in [15] and for integer in [16] linear bilevel problems, but it can be easily adapted to linear bilevel problems. The same holds true for the following surveyed results.

In [15], 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 problem is infeasible, unbounded, or finite optimal [15] (see Example 3 for an unbounded bilevel model with bounded upper-level variables). Furthermore, it is shown in [17] 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 problem 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 problem. One of the main drawback of both these works [15, 17] in the study of unboundedness is the assumption that some of the variables are explicitly bounded, restricting the possible scenarios leading to an unbounded bilevel problem to unboundedness arising in the lower-level problem. Finally, the watermelon algorithm presented in [16] to solve integer bilevel problems can provide a certificate of unboundedness, when one exists. This algorithm is based on a branch-and-bound approach which uses multi-way disjunctive cuts to eliminate bilevel infeasible solutions from the search space. This approach cannot be extended to linear bilevel optimization, because the designed sets of infeasible points rely on the feasible region being disconnected, a property enforced by integrality constraints. Moreover the branch-and-bound applied to the variables would also not be directly adaptable to a linear continuous framework.

1.2 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 address this gap and close important open questions with our main contribution being from a theoretical computational complexity perspective. Jeroslow's ground-breaking work [4] establishes that the complexity of determining if a multi-level model admits an optimal solution rises one level in the polynomial hierarchy for each additional level added. Complementing this seminal work, we show the hardness of deciding unboundedness in multilevel problems. Additionally, we present two algorithmic approaches for dealing with unboundedness from a practical perspective.

The remainder of this paper is organised as follows. In Section 2, we show that the decision problem of whether a linear bilevel problem is unbounded is strongly NP-complete, and draw some parallels to the pessimistic bilevel formulation. More generally, we also show that checking unboundedness of a linear multilevel problem with k levels is Σ_{k-1}^p-hard in Section 3. In this section, we also show the Σ_k^p-hardness of deciding unboundedness of a mixed-integer k-level problem. In Section 4, 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, and present a brief computational comparison. Finally, in Section 5, we summarise our contributions, and propose directions for future research.

2 Computational Complexity of Checking Unboundedness

We formalize the problem of deciding the unboundedness of a bilevel problem in Section 2.1. Then, in Section 2.2, we show that the problem is NP-complete for the optimistic bilevel formulation, and in Section 2.3, we show the problem's NP-hardness for the pessimistic bilevel formulation.

2.1 Decision Problem

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

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

is unbounded 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 [18]. However, this question can be simplified into one with only an existential quantifier as:

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

Therefore, this allows 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 [19], 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.

We know that a linear 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, in linear bilevel optimization, 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. Condition (2) ensures that every point on the half-line generated by the feasible solution (x, y) and the direction $(\Delta x, \Delta y)$ is a feasible solution for the bilevel problem, and condition (3) that the upper-level objective value improves along this half-line. 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 satisfy (2)-(3)?

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

2.2 NP-completeness of Optimistic 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 [20].

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:

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

where $\mathcal{F}_D = \{\lambda : D^\top \lambda = -f; \lambda \geq 0\}$ is the feasible set of the dual of the lower-level problem.

Proof From [20, 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 [20], 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. □

Theorem 2 *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.*

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

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

To prove the opposite implication, we assume that (P) is unbounded and, by contradiction, that for all $\omega \in \{1,2\}^{n_2}$ (P_ω) 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_ω) is unbounded. We have proved both implications as required. □

Given Lemma 1 and Theorem 2, we conclude that the question of UNBOUNDED-BLP can be equivalently expressed 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 [19]. Therefore, this problem belongs to the complexity class NP [18]. 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 by proving that it is also strongly NP-hard. We show this result for problems without linking constraints. We present a similar result for bilevel problems with linking constraints in Appendix A, whose proof is useful for building intuition for the multilevel linear case in Section 3.1.

In order to prove this result, we derive a reduction from the decision version of the 3-SAT problem known to be NP-complete [21].

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

Theorem 3 *UNBOUNDED-BLP without linking constraints is strongly NP-complete.*

Proof From Lemma 1 and Theorem 2, 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 ($\bar{\mathrm{B}}$) is unbounded.

$$\begin{aligned} \min_{x,y,z,w} \quad & \sum_{i=1}^{n} z_i - \frac{1}{2n}\sum_{i=1}^{n} w_i && (\bar{\mathrm{B}}) \\ \text{s.t.} \quad & A_{\mathrm{S}} x + y \geq \frac{3}{2} + c_{\mathrm{S}}, \\ & \frac{1}{2} - y \leq x_i \leq \frac{1}{2} + y \quad \forall i \in \{1,\dots,n\}, \end{aligned}$$

$$
\begin{aligned}
(z, w) \in \arg\max_{\bar{z},\bar{w}} \quad & \sum_{i=1}^{n} z_i - \frac{1}{2n}\sum_{i=1}^{n} w_i \\
\text{s.t.} \quad & z_i \leq y - \frac{1}{2} + x_i \quad \forall i \in \{1, \dots, n\}, \\
& z_i \leq y - x_i + \frac{1}{2} \quad \forall i \in \{1, \dots, n\}, \\
& w_i \geq x_i - \frac{1}{2} \quad \forall i \in \{1, \dots, n\}, \\
& w_i \geq \frac{1}{2} - x_i \quad \forall i \in \{1, \dots, n\}.
\end{aligned}
$$

Note that the problem ($\bar{\text{B}}$) is always feasible, because $y = 0$, $x_i = \frac{1}{2}$ $\forall i \in \{1, \dots, n\}$, $z = w = \mathbf{0}$ is a feasible solution. Furthermore, for any given upper-level decisions y and x, the lower-level optimal solution is given by:

$$
\begin{aligned}
z_i &= \min\left\{y - \frac{1}{2} + x_i;\ y - x_i + \frac{1}{2}\right\} = y - \left|x_i - \frac{1}{2}\right| \quad \forall i \in \{1, \dots, n\}, \\
w_i &= \max\left\{x_i - \frac{1}{2};\ \frac{1}{2} - x_i\right\} = \left|x_i - \frac{1}{2}\right| \quad \forall i \in \{1, \dots, n\}.
\end{aligned}
$$

Proof of if. Assume that 3-SAT is a YES instance, then S is satisfiable and we know that $\exists a \in \{0, 1\}^n$ such that $A_{\text{S}} a \geq 1 + c_{\text{S}}$.

Let $y \geq 0$, and build

$$
x = \begin{cases} \frac{1}{2} - y & \text{if } a_i = 0 \\ \frac{1}{2} + y & \text{if } a_i = 1 \end{cases}, \quad z = \mathbf{0}, \quad w_i = y \ \forall i \in \{1, \dots, n\}.
$$

First, we show that for all $y \geq 0$, this yields a feasible solution of problem ($\bar{\text{B}}$). Since $x \in \left\{\frac{1}{2} - y, \frac{1}{2} + y\right\}^n$, it is straightforward to verify that this solution is optimal for the lower-level problem, and that it verifies the upper-level constraint:

$$
\frac{1}{2} - y \leq x_i \leq \frac{1}{2} + y.
$$

Therefore, we must only show that it also verifies $A_{\text{S}} x + y \geq \frac{3}{2} + c_{\text{S}}$. Note that for each clause $t \in S$, there are exactly three literals $\bar{s}_{t1}$, $\bar{s}_{t2}$, $\bar{s}_{t3}$ such that:

$$
(A_{\text{S}} x - c_{\text{S}})_t = \bar{s}_{t1} + \bar{s}_{t2} + \bar{s}_{t3},
$$

where for all $j \in \{1, 2, 3\}$, there exists $i \in \{1, \dots, n\}$ such that $\bar{s}_{tj}$ is either x_i or $1 - x_i$. From the bounds on x, we know that:

$$
x_i, 1 - x_i \geq \frac{1}{2} - y \ \forall i \in \{1, \dots, n\} \Rightarrow \bar{s}_{tj} \geq \frac{1}{2} - y \ \forall j \in \{1, 2, 3\}. \tag{5}
$$

Furthermore, since a is a true assignment, then at least of its literals in clause $t \in S$ is true, this is $\exists j \in \{1, 2, 3\} : s_{tj} = 1$, where $(A_{\text{S}} a - c_{\text{S}})_t = s_{t1} + s_{t2} + s_{t3}$. This implies that the corresponding literal in the x variables is $\frac{1}{2} + y$:

$$
\exists j \in \{1, 2, 3\} : \bar{s}_{tj} = \frac{1}{2} + y. \tag{6}
$$

From equations (5) and (6), we obtain:

$$
(A_{\text{S}} x - c_{\text{S}})_t \geq \left(\frac{1}{2} - y\right) + \left(\frac{1}{2} - y\right) + \left(\frac{1}{2} + y\right) = \frac{3}{2} - y.
$$

Since this holds true for any clause $t \in S$, then for all $y \geq 0$, the solution we build is feasible for problem ($\bar{\text{B}}$).

In addition, the upper-level objective value at these solutions is:

$$\sum_{i=1}^{n} z_i - \frac{1}{2n}\sum_{i=1}^{n} w_i = -\frac{1}{2}y.$$

Consequently, we can create a sequence of feasible points with decreasing (improving) objective value, by picking $y \in \{0, 1, 2, \dots\}$, and the corresponding x, z, and w values. Thus, problem ($\bar{\mathrm{B}}$) is unbounded.

Proof of only if. Assume that problem ($\bar{\mathrm{B}}$) is unbounded. Then, there is a feasible point $(\bar{y}, \bar{x}, \bar{z}, \bar{w})$ and a direction of unboundedness $(\Delta y, \Delta x, \Delta z, \Delta w)$ at that point. Since ($\bar{\mathrm{B}}$) is a minimization problem, we know that the objective value decreases along $(\bar{y}, \bar{x}, \bar{z}, \bar{w}) + k(\Delta y, \Delta x, \Delta z, \Delta w)$ towards $-\infty$, as $k \to +\infty$. In particular, we know that there is a $\bar{k} > 0$ such that $(y, x, z, w) = (\bar{y}, \bar{x}, \bar{z}, \bar{w}) + \bar{k}(\Delta y, \Delta x, \Delta z, \Delta w)$ is a feasible point with strictly negative upper-level objective value:

$$\sum_{i=1}^{n} z_i - \frac{1}{2n}\sum_{i=1}^{n} w_i < 0.$$

We now show that the assignment:

$$a_i = \begin{cases} 0 & \text{if } x_i \leq \frac{1}{2} \\ 1 & \text{if } x_i > \frac{1}{2} \end{cases}$$

is a true assignment of S.

In order to do so, we start by showing that, since the feasible point (y, x, z, w) has strictly negative objective value, then for all clauses $t \in S$, at least one of the literals has value strictly greater than $\frac{1}{2}$, this is:

$$\forall t \in S,\ \exists j \in \{1, 2, 3\} : \bar{s}_{tj} > \frac{1}{2},$$

where $(A_{\mathrm{S}}x - c)_t = \bar{s}_{t1} + \bar{s}_{t2} + \bar{s}_{t3}$. First, since $A_{\mathrm{S}}x + y \geq \frac{3}{2} + c$, we know that for each clause $t \in S$, there exists $j \in \{1, 2, 3\}$ such that the corresponding literal $\bar{s}_{tj} \geq \frac{1}{2} - \frac{y}{3}$ where $A_{\mathrm{S}}x - c = \bar{s}_{t1} + \bar{s}_{t2} + \bar{s}_{t3}$. If, by contradiction, all literals $\bar{s}_{t1}, \bar{s}_{t2}, \bar{s}_{t3} < \frac{1}{2} - \frac{y}{3}$, then $A_{\mathrm{S}}x - c < \frac{3}{2} - y$ which implies that (x, y, z, w) is not feasible.

Now, assume, by contradiction, that all literals $\bar{s}_{t1}, \bar{s}_{t2}, \bar{s}_{t3} \leq \frac{1}{2}$. We know already that there exists $j \in \{1, 2, 3\}$ such that $\bar{s}_{tj} \geq \frac{1}{2} - \frac{y}{3}$, let x_p be the corresponding variable. Then, we can deduce that:

$$\begin{aligned} \sum_{i=1}^{n} z_i - \frac{1}{2n}\sum_{i=1}^{n} w_i &= \sum_{i=1}^{n}\left[y - \left|x_i - \frac{1}{2}\right|\right] - \frac{1}{2n}\sum_{i=1}^{n}\left|x_i - \frac{1}{2}\right|, \\ &\geq y - \left|x_p - \frac{1}{2}\right| - \frac{1}{2n}ny, \\ &\geq y - \frac{1}{3}y - \frac{1}{2}y, \\ &= \frac{2}{3}y \geq 0, \end{aligned}$$

where the first inequality holds true, because $x_i \in \left[\frac{1}{2} - y, \frac{1}{2} + y\right]$ implies $\left|x_i - \frac{1}{2}\right| \leq y$. The second inequality holds true, because $\bar{s}_{tj} \in \left[\frac{1}{2} - \frac{y}{3}, \frac{1}{2}\right]$ implies $\left|x_p - \frac{1}{2}\right| \leq \frac{y}{3}$. In fact, if $\bar{s}_{tj} = x_p$, then $x_p \in \left[\frac{1}{2} - \frac{y}{3}, \frac{1}{2}\right]$, and if $\bar{s}_{tj} = 1 - x_p$, then $x_p \in \left[\frac{1}{2}, \frac{1}{2} + \frac{y}{3}\right]$. In both cases, we know that $\left|x_i - \frac{1}{2}\right| \in \left[0, \frac{y}{3}\right]$. The final inequality holds true, because for a feasible solution $x \in \left[\frac{1}{2} - y, \frac{1}{2} + y\right]^n$ to exist, we must have $y \geq 0$. This inequality contradicts the fact that

(y, x, z, w) has strictly negative objective value, thus we conclude that for each clause $t \in S$, there exists $j \in \{1, 2, 3\}$ such that the corresponding literal $\bar{s}_{tj} > \frac{1}{2}$.

Now, we are ready to conclude the proof by showing that a is a true assignment of S. Let x_p be the variable associated with that literal. If $\bar{s}_{tj} = x_p$, then $s_{tj} = a_p = 1$. If $\bar{s}_{tj} = 1 - x_p$, then $x_p > \frac{1}{2}$, $a_p = 0$ and $s_{tj} = 1 - a_p = 1$.

In any case, we obtain:

$$(A_{\mathrm{S}} a - c_{\mathrm{S}})_t = s_{t1} + s_{t2} + s_{t3} \geq 1.$$

Since, this holds true for any clause $t \in S$, then $a \in \{0, 1\}^n$ verifies $A_{\mathrm{S}} a \geq 1 + c_{\mathrm{S}}$, and the 3-SAT is a YES instance. □

2.3 NP-hardness of Pessimistic Bilevel Case

So far we have considered the optimistic formulation of a linear bilevel problem. Another possible formulation is the pessimistic one, in which, if there are multiple lower-level optimal solutions, the worst solution with respect to the upper-level will be selected. In the presence of linking constraints, this might mean that for a given upper-level decision, the follower selects an optimal lower-level solution that violates the linking constraints, leading to infeasibility of the selected upper-level decision.

We can equivalently formulate the optimistic problem formulation as:

$$\min_{x \in \mathcal{X}} \min_{y \in \mathcal{S}(x)} \quad c^\top x + d^\top y,$$

where $\mathcal{X} = \{x : \exists y \in \mathcal{S}(x) : Ax + By \leq a\}$ is the set of feasible upper-level variables, and $\mathcal{S}(x) = \arg\min_{\tilde{y}} \left\{ f^\top \tilde{y} : Cx + D\tilde{y} \leq b \right\}$ is the set of optimal solutions of the lower-level problem at x. Given this notation, we define the pessimistic formulation, similarly to [23], as:

$$\min_{x \in \mathcal{X}} \max_{y \in \mathcal{S}(x)} \quad c^\top x + d^\top y. \tag{P}$$

The underlying assumption in both formulations is that for a solution (x, y) to be bilevel feasible, the lower-level problem cannot be infeasible, i.e. $\mathcal{S}(x) \neq \emptyset$. This assumption is not always considered and an alternative approach for the pessimistic formulation is presented by Wiesemann et al. [24]. Finally, note that problem (P) can be rewritten as:

$$\begin{aligned} \min_{x \in \mathcal{X}} \min_{y \in \mathcal{S}(x)} \quad & c^\top x + d^\top y \\ \text{s.t.} \quad & c^\top x + d^\top y \geq c^\top x + d^\top \bar{y} \quad \forall \bar{y} \in \mathcal{S}(x). \end{aligned} \tag{P'}$$

In general, unboundedness of the optimistic formulation of a bilevel problem does not imply that of its pessimistic formulation, as illustrated in Example 1.

Example 1 (Unboundedness in Optimistic vs Pessimistic Formulations) Consider the following bilevel problem:

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

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 $(\Delta x, \Delta y_1, \Delta y_2) = (1, 0, 1)$ 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.

Nevertheless, the NP-hardness part of Theorem 3 still holds if we consider a pessimistic formulation, because the lower-level optimal solutions 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, even without linking constraints:

Corollary 4 *Deciding whether the pessimistic linear bilevel program* (P') *is unbounded is strongly NP-hard.*

Even though we have seen in Example 1 that unboundedness of the optimistic formulation of a bilevel problem does not imply that of its pessimistic formulation, the converse is true. To conclude this section, we show that the boundedness of the optimistic formulation of a bilevel problem implies that of its pessimistic formulation in Lemma 5.

Lemma 5 *If the pessimistic formulation (P') is unbounded, then the corresponding optimistic formulation (B) is also unbounded.*

Proof The optimistic formulation (B) is a relaxation of the pessimistic one (P'), because the feasible set of the pessimistic formulation is the feasible set of the optimistic formulation plus one new set of constraints. Consequently, the optimal value of the pessimistic formulation (P') is an upper bound on the optimal value of the optimistic model (B). Therefore, if the pessimistic formulation (P') is unbounded, i.e. has optimal value $-\infty$, then so does the optimistic formulation (B). □

3 Complexity Results in Multilevel Optimization

In this section, we extend our results to multilevel optimization by showing that deciding whether a linear k-level optimization problem is unbounded is Σ^p_{k-1}-hard in Section 3.1, and that deciding whether a mixed-integer k-level optimization problem is unbounded is Σ^p_k-hard in Section 3.2.

3.1 Linear Multilevel Optimization

We have already showed that for $k = 2$, checking if a bilevel problem is unbounded is NP-hard, or equivalently Σ^p_1-hard. In this section, we extend this result to show 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 linear k-level problem (KLP):

$$\begin{aligned}\min_{x}\ & f_k^\top x\\ \text{s.t. }\ & x \in C^k\\ & x^{(k-1)} \in \arg\min_{x^{(k-1)}}\ f_{k-1}^\top x^{(k-1)}\\ &\qquad \text{s.t. }\ x^{(k-1)} \in C^{k-1}\\ &\qquad\qquad x^{(k-2)} \in \arg\min_{x^{(k-2)}}\ (\dots)\\ &\qquad\qquad\qquad \vdots\\ &\qquad\qquad x^{(2)} \in \arg\min_{x^{(2)}}\quad f_2^\top x^{(2)}\\ &\qquad\qquad\qquad \text{s.t.}\quad x^{(2)} \in C^2\\ &\qquad\qquad\qquad\qquad x^{(1)} \in \arg\min_{x^{(1)}}\ f_1^\top x^{(1)}\\ &\qquad\qquad\qquad\qquad\qquad \text{s.t. }\ x^1 \in C^1\end{aligned} \tag{KLP}$$

where $x = (x^1, \dots, x^k)$ are the decision variables, and C^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 C^i is parametrised by the variables of all the levels above i, so the notation C^i is an abbreviation for $C^i(x^{i+1}, \dots, x^k)$. The subset of decision variables of level i is $x^{(i)} = (x^1, \dots, x^i)$, and f_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: $f_k, \dots, f_1$ rational vectors of appropriate dimension and $C^k, \dots, C^1$ linear polyhedra (defined by rational coefficients).
QUESTION: Is the corresponding k-level model unbounded?

In Theorem 6, we show that UNBOUNDED-KLP is strongly Σ^p_{k-1}-hard.

Theorem 6 *UNBOUNDED-KLP is Σ^p_{k-1}-hard.*

We have divided the proof of Theorem 6 into smaller sub-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. Thus, this proof can be obtained by combining Theorem 7, Theorem 8 and Theorem 9 presented in the remainder of this section.

The decision problem that we use in all the sub-proofs of Theorem 6 is the $(k-1)$-ALTERNATING QUANTIFIED SATISFIABILITY with k adjusted as suited. This decision problem is known to be Σ^p_{k-1}-complete [25].

$(k-1)$-Alternating Quantified Satisfiability:
INSTANCE: Disjoint non-empty sets of variables $X_1, \dots, X_{k-1}$, 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 $c \in S$.
QUESTION:

- When k odd, $(\mathcal{B}_{k-1} \cap \overline{3\text{CNF}})$: 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, $(\mathcal{B}_{k-1} \cup 3\text{CNF})$: 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?

Following similar notation to the one used for the 3-SAT problem, we say that $\mathcal{B}_{k-1} \cap \overline{3\text{CNF}}$ (for k odd) is a YES instance if and only if $\exists a_{k-1} \in \{0,1\}^{n_{k-1}}$, $\forall a_{k-2} \in \{0,1\}^{n_{k-2}}$, $\dots$, $\exists a_2 \in \{0,1\}^{n_2}$, $\forall a_1 \in \{0,1\}^{n_1}$ such that

$$\sum_{l=1}^{k-1} A_l a_l \ngeq 1 + c,$$

where $A_l \in \{-1,0,1\}^{m \times n_l}$ with $m = |S|$ the number of clauses in S, and $n_l = |X_l|$ for $l \in \{1, \dots, k-1\}$, and $c \in \{-3,-2,-1,0\}^m$.

Similarly, we say that $\mathcal{B}_{k-1} \cup \text{3CNF}$ (for k even) is a YES instance if an only if $\exists a_{k-1} \in \{0,1\}^{n_{k-1}}$, $\forall a_{k-2} \in \{0,1\}^{n_{k-2}}$, $\ldots$, $\forall a_2 \in \{0,1\}^{n_2}$, $\exists a_1 \in \{0,1\}^{n_1}$ such that

$$\sum_{l=1}^{k-1} A_l a_l \geq 1 + c.$$

3.1.1 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 7.

Theorem 7 *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:

$$\begin{aligned}
\max_{\substack{y, x_2, x_1, \\ s, z}} \quad & y \\
\text{s.t.} \quad & y \geq 1, \\
& x_2 \in [0, y]^{n_2}, \\
& z_2 = \mathbf{0}, \\
& s = 0, \\
& (x_1, s, z) \in \arg\max_{x_1, s, z} \; s \\
& \qquad \text{s.t.} \; \sum_{i=1}^{2} A_i x_i \geq s + cy, \\
& \qquad \qquad x_1 \in [0, y]^{n_1}, \\
& \qquad \qquad z_1 = \mathbf{0}, \\
& \qquad \qquad s \in [0, y], \\
& \qquad \qquad z_s = 0, \\
& \qquad \qquad z \in \arg\max_{z} \; z_s + \sum_{l=1}^{2} \sum_{i=1}^{n_l} (z_l)_i \\
& \qquad \qquad \quad \text{s.t.} \; z_l \leq x_l \quad \forall l \in \{1, 2\}, \\
& \qquad \qquad \qquad z_l \leq y - x_l \quad \forall l \in \{1, 2\}, \\
& \qquad \qquad \qquad z_s \leq s, \\
& \qquad \qquad \qquad z_s \leq y - s,
\end{aligned} \tag{3LP}$$

where we abbreviate $z = (z_1, z_2, z_s)$, and for $l \in \{1, 2\}$ denote n_l as the dimension of x_l. Note that optimality of level 1 implies that any feasible solution satisfies $(z_1)_i = \min\{(x_1)_i, y - (x_1)_i\}$ $\forall i \in \{1, \ldots, n_1\}$, $(z_2)_i = \min\{(x_2)_i, y - (x_2)_i\}$ $\forall i \in \{1, \ldots, n_2\}$ and $z_s = \min\{s, y - s\}$. In addition, the linking constraints $z_2 = \mathbf{0}$, $z_1 = \mathbf{0}$, $z_s = 0$ at levels 3 and 2 enforce that $x_2 \in \{0, y\}^{n_2}$, $x_1 \in \{0, y\}^{n_1}$ and $s \in \{0, y\}$, respectively. It is important that these linking constraints appear in the level that decides on the corresponding variables (x_2, x_1 and s) whose integrality is being enforce.

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 $\mathcal{B}_2 \cap \overline{3\text{CNF}}$ is a YES instance, this is that $\exists \bar{a}_2 \in \{0,1\}$, $\forall a_1 \in \{0,1\} : A_1 a_1 + A_2 a_2 \not\geq 1 + c$.

Let $y \geq 1$, and $x_2 = \bar{a}_2 y$, and $a_1 \in \{0,1\}^{n_1}$. We show that (y, x_2) along with $x_1 = a_1 y$, $s = 0$, $z_1 = z_2 = \mathbf{0}$ and $z_s = 0$ constitutes a feasible solution of (3LP). It is easy to verify that the feasibility constraints at all levels are verified. According to our observation about optimal solutions for level 1, it is clear that this solution $(z_1, z_2, z_s) = (\mathbf{0}, \mathbf{0}, 0)$ is optimal for level 1. We show that this solution is also optimal for level 2 by contradiction. Assume, by contradiction, that $s = y$ would be feasible for level 2. Then,

$$\sum_{i=1}^{2} A_i x_i \geq s + cy \Leftrightarrow A_2 \bar{a}_2 + A_1 a_1 \geq 1 + c,$$

where the equivalence arises from $y \geq 1$. This contradicts our assumption that $\mathcal{B}_2 \cap \overline{3\text{CNF}}$ is a YES instance. We also note that any assignment $a_2 \in \{0,1\}^{n_2}$, $a_1 \in \{0,1\}^{n_1}$ satisfies $A_1 a_1 + A_2 a_2 \geq c$, so $s = 0$ is always feasible for level 2. Therefore, the problem at level 2 has optimal value 0, and the solution considered is optimal. Since the solution we build is feasible for any $y \geq 1$, then by setting $y \in \{1, 2, 3, ...\}$ we can build a sequence of feasible points for (3LP) which have increasing objective value y. Therefore, the trilevel problem (3LP) is unbounded.

Proof of only if. Assume that $\mathcal{B}_2 \cap \overline{3\text{CNF}}$ is a NO instance, this is that $\neg(\exists a_2 \in \{0,1\}^{n_2}, \forall a_1 \in \{0,1\}^{n_1} : A_1 a_1 + A_2 a_2 \not\geq 1 + c)$. Equivalently, we can write:

$$\forall a_2 \in \{0,1\}^{n_2}, \exists a_1 \in \{0,1\}^{n_1} : A_1 a_1 + A_2 a_2 \geq 1 + c.$$

We show that (3LP) is infeasible. Assume, by contradiction, that there is a feasible solution $(y, x_1, x_2, s, z_1, z_2, z_s)$ of (3LP). Let $a_2 = \frac{1}{y} x_2$. Since $x_2 \in \{0, y\}^{n_2}$, then $a_2 \in \{0,1\}^{n_2}$. By assumption, we know that there exists $a_1 \in \{0,1\}^{n_1}$ such that $A_1 a_1 + A_2 a_2 \geq 1 + c$. Therefore, for y and x_2 fixed, $\bar{x}_1 = a_1 y$, $\bar{s} = y$, $\bar{z}_1 = \bar{z}_2 = \mathbf{0}$ and $\bar{z}_s = 0$ is an optimal solution of the problem at level 2. This implies that the optimal value of level 2 for (y, x_2) is y, and consequently any other optimal solution must have the s variable set to y. Then, our feasible solution has $s = y$. This however violates the linking constraint $s = 0$, so the solution cannot be feasible by contradiction. By arbitrariness of the choice of feasible solution, we conclude that (3LP) is infeasible. Hence, the 3-level problem (3LP) is not unbounded. □

3.1.2 Unbounded-KLP with Odd k is Σ^p_{k-1}-hard

Throughout this section, we assume that $k \geq 4$ is an odd number. Based on the $(k-1)$-Alternating Quantified Satisfiability ($\mathcal{B}_{k-1} \cap \overline{3\text{CNF}}$) problem, we show that Unbounded-KLP where k is odd is a Σ^p_{k-1}-hard problem in Theorem 8.

Theorem 8 *Unbounded-KLP for k odd is Σ^p_{k-1}-hard.*

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

$$
\begin{aligned}
\max_{y,x,s,z} \quad & y \\
\text{s.t.} \quad & y \geq 1, \\
& x_{k-1} \in [0, y]^{n_{k-1}}, \\
& z_{k-1} = \mathbf{0}, \\
& s = 0, \\
& \qquad \vdots \\
l \text{ odd: } & (x^{(l)}, s, z) \in \arg\max_{x^{(l)}, s, z} \left\{ s : x_l \in [0, y]^{n_l}; z_l = \mathbf{0};\ (x^{(l-1)}, s, z) \in \Phi^{l-1} \right\}, \\
l \text{ even: } & (x^{(l)}, s, z) \in \arg\min_{x^{(l)}, z} \left\{ s : x_l \in [0, y]^{n_l}; z_l = \mathbf{0};\ (x^{(l-1)}, s, z) \in \Phi^{l-1} \right\}, \\
& \qquad \vdots \\
& (x_1, s, z) \in \arg\max_{x_1, s, z} \quad s \\
& \qquad \text{s.t.} \quad \sum_{i=1}^{k-1} A_i x_i \geq s + cy, \\
& \qquad\qquad x_1 \in [0, y]^{n_1}, \\
& \qquad\qquad z_1 = \mathbf{0}, \\
& \qquad\qquad s \in [0, y], \\
& \qquad\qquad z_s = 0, \\
& \qquad\qquad z \in \arg\max_{z} z_s + \sum_{l=1}^{k-1} \sum_{i=1}^{n_l} (z_l)_i \\
& \qquad\qquad\qquad \text{s.t.} \quad (z_l)_i \leq (x_l)_i \qquad \forall l,\ \forall i, \\
& \qquad\qquad\qquad\qquad (z_l)_i \leq y - (x_l)_i \qquad \forall l,\ \forall i, \\
& \qquad\qquad\qquad\qquad z_s \leq s, \\
& \qquad\qquad\qquad\qquad z_s \leq y - s,
\end{aligned}
\tag{Odd-KLP}
$$

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 parametrised by the variables $(y, x_{k-1}, \ldots, x_{i+1})$ of the levels above.

Note that, for $l \leq k-2$, the problem at level l is never unbounded because y is a decision of level $k-1$ and hence a parameter for this level. Optimality of level 1 implies that at any feasible solution we have that $(z_l)_i = \min\{(x_l)_i, y - (x_l)_i\}\ \forall l \in \{1, \ldots, k-1\}, \forall i \in \{1, \ldots, n_l\}$ and $z_s = \min\{s, y - s\}$. In addition, the linking constraints $z_l = \mathbf{0}\ \forall l \in \{1, \ldots, k-1\}$ and $z_s = 0$ at each level enforce that for $l \in \{1, \ldots, k-1\} : x_l \in \{0, y\}^{n_l}$ and $s \in \{0, y\}$, respectively. Note also that $s = 0$ is always feasible for level 2, since any set of assignment values $a_l \in \{0, 1\}^{n_l}$ for $l \in \{1, \ldots, k-1\}$ satisfies $\sum_{i=1}^{k-1} A_i a_i \geq c$.

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

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

Let $y \geq 1$, and $x_{k-1} = a_{k-1} y$, where a_{k-1} is the assignment we know exists by assumption. Let $x_l = a_l y$ for all $l \in \{k-2, \ldots, 1\}$, where for l odd $a_l \in \{0, 1\}^{n_l}$ can be any assignment, and for l even a_l is the assignment we know exists by assumption and which depends on the choice of a_{l+1}. We show that this choice of (y, x) along with $s = 0$, $z_l = \mathbf{0}$ for $l \in \{k-1, \ldots, 1\}$ and $z_s = 0$ constitutes a feasible solution of (Odd-KLP).

It is easy to verify that the feasibility constraints at all levels are verified. According to our observation about optimal solutions for level 1, it is clear that this solution $z_l = \mathbf{0}$ for $l \in \{k-1, \ldots, 1\}$ and $z_s = 0$ is optimal for level 1. We must also show each x_l and s are optimal for the corresponding levels.

Let $l \in \{1, \ldots, k-2\}$. For even l, since we selected x_l as this solution which we know exists (by assumption), then independently of what the following levels associated with an odd l value chose, $s = 0$ is always the only feasible choice for s at level 2. This setting of $s = 0$ minimizes the objective value s at this level where x_l for even l, is decided on. For odd l, independently of which x_l values are picked at this level, there will always be a corresponding solution for the following levels associated with an even l value, which will enforce $s = 0$ in order for the assignment constraint to hold. In both cases, the selected x_l values and $s = 0$ are optimal decisions for the corresponding levels.

Since the solution we build is feasible for any $y \geq 1$, then by setting $y \in \{1, 2, 3, ...\}$ we can build a sequence of feasible points for (Odd-KLP) which have increasing/improving objective value y. Therefore, the k-level problem (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 $\neg(\exists a_{k-1} \in \{0,1\}^{n_{k-1}}, \ \ldots, \ \exists a_2 \in \{0,1\}^{n_2}, \ \forall a_1 \in \{0,1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l \not\geq 1 + c)$. Equivalently, we can write:

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

We show that (Odd-KLP) is infeasible. Assume, by contradiction, that there is a feasible solution $(y, x_{k-1}, \ldots, x_1, s, z_{k-1}, \ldots, z_1, z_s)$ of (Odd-KLP).

Let $a_{k-1} = \frac{1}{y} x_{k-1}$. Since $x_{k-1} \in \{0, y\}^{n_{k-1}}$, then $a_{k-1} \in \{0,1\}^{n_{k-1}}$. Then, we show that $s = y$. Let $l \in \{1, \ldots, k-2\}$. For odd l, the corresponding level maximizes s, and $x_l = a_l y$ is an feasible solution that allows for $s = y$ to be selected. Therefore, the optimal objective value of this level is y, corresponding to a solution $s = y$ at level 2. For even l, independently of the solution selected by the corresponding level, the following levels associated with an odd l value always chose a solution that makes $s = y$ the optimal at level 2.

This value of s however violates the linking constraint $s = 0$, so the solution cannot be feasible, and we have reached a contradiction. By arbitrariness of the choice of feasible solution, we conclude that (Odd-KLP) is infeasible. Hence, the k-level problem (Odd-KLP) is not unbounded. □

3.1.3 Unbounded-KLP with Even k is Σ^p_{k-1}-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^p_{k-1}-hard problem in Theorem 9.

Theorem 9 *Unbounded-KLP for k even is Σ^p_{k-1}-hard.*

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

$$
\begin{aligned}
\max_{y,x,s,z} \quad & y \\
\text{s.t.} \quad & y \geq 1, \\
& x_{k-1} \in [0, y]^{n_{k-1}}, \\
& z_{k-1} = \mathbf{0}, \\
& s = y, \\
& \qquad \vdots \\
l \text{ even: } & (x^{(l)}, s, z) \in \arg\min_{x^{(l)}, z} \left\{ s : x_l \in [0, y]^{n_l}; z_l = \mathbf{0};\ (x^{(l-1)}, s, z) \in \Phi^{l-1} \right\}, \\
l \text{ odd: } & (x^{(l)}, s, z) \in \arg\max_{x^{(l)}, s, z} \left\{ s : x_l \in [0, y]^{n_l}; z_l = \mathbf{0};\ (x^{(l-1)}, s, z) \in \Phi^{l-1} \right\}, \\
& \qquad \vdots \\
& (x_1, s, z) \in \arg\max_{x_1, s, z} \quad s \\
& \qquad \text{s.t.} \quad \sum_{i=1}^{k-1} A_i x_i \geq s + cy, \\
& \qquad \qquad x_1 \in [0, y]^{n_1}, \\
& \qquad \qquad z_1 = \mathbf{0}, \\
& \qquad \qquad s \in [0, y], \\
& \qquad \qquad z_s = 0, \\
& \qquad \qquad z \in \arg\max_{z} z_s + \sum_{l=1}^{k-1} \sum_{i=1}^{n_l} (z_l)_i \\
& \qquad \qquad \qquad \text{s.t.} \quad (z_l)_i \leq (x_l)_i \qquad \forall l,\ \forall i, \\
& \qquad \qquad \qquad \qquad (z_l)_i \leq y - (x_l)_i \qquad \forall l,\ \forall i, \\
& \qquad \qquad \qquad \qquad z_s \leq s, \\
& \qquad \qquad \qquad \qquad z_s \leq y - s,
\end{aligned}
\tag{Even-KLP}
$$

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 parametrised by the variables $(y, x_{k-1}, \ldots, x_{i+1})$ of the levels above. This problem (Even-KLP) is similar to the reduction problem (Odd-KLP) used in the proof for odd k, where the constraint $s = 0$ is replaced with $s = y$.

Note that, for $l \leq k-2$, the problem at level l is never unbounded because y is a decision of level $k-1$ and hence a parameter for this level. Optimality of level 1 implies that at any feasible solution we have that $(z_l)_i = \min\{(x_l)_i, y-(x_l)_i\}$ $\forall l \in \{1, \ldots, k-1\}, \forall i \in \{1, \ldots, n_l\}$ and $z_s = \min\{s, y-s\}$. In addition, the linking constraints $z_l = \mathbf{0}$ $\forall l \in \{1, \ldots, k-1\}$ and $z_s = 0$ at level k enforce that for $l \in \{1, \ldots, k-1\} : x_l \in \{0, y\}^{n_l}$ and $s \in \{0, y\}$, respectively. Note also that $s = 0$ is always feasible for level 2, since any set of assignment values $a_l \in \{0,1\}^{n_l}$ for $l \in \{1, \ldots, k-1\}$ satisfies $\sum_{i=1}^{k-1} A_i a_i \geq c$.

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

Let $y \geq 1$, and $x_{k-1} = a_{k-1} y$, where a_{k-1} is the assignment we know exists by assumption. Let $x_l = a_l y$ for all $l \in \{k-2, \ldots, 1\}$, where for l even $a_l \in \{0,1\}^{n_l}$ can be any assignment, and for l odd a_l is the assignment we know exists by assumption and which depends on the choice of a_{l+1}. We show that this choice of (y, x) along with $s = y$, $z_l = \mathbf{0}$ for $l \in \{k-1, \dots, 1\}$ and $z_s = 0$ constitutes a feasible solution of (Even-KLP).

It is easy to verify that the feasibility constraints at all levels are verified. According to our observation about optimal solutions for level 1, it is clear that this solution $z_l = \mathbf{0}$ for $l \in \{k-1, \dots, 1\}$ and $z_s = 0$ is optimal for level 1. We must also show each x_l and s are optimal for the corresponding levels.

Let $l \in \{1, \dots, k-2\}$. For odd l, the corresponding level whose goal is to maximise s will choose $x_l = a_l y$ as the assignment that results in $s = y$ being feasible (and hence optimal) for level 2. We know, by assumption, that such a decision exists independently of what the following levels associated with an even l value chose x_l to be. For even l, independently of the x_l selected, we know the following levels associated with an odd l value will select the decision that lead to $s = y$. In both cases, the selected x_l values and $s = y$ are optimal decisions for the corresponding levels. Since the solution we build is feasible for any $y \geq 1$, then by setting $y \in \{1, 2, 3, ...\}$ we can build a sequence of feasible points for (Even-KLP) which have increasing/improving objective value y. Therefore, the k-level problem (Even-KLP) is unbounded.

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

$$\forall a_{k-1} \in \{0,1\}^{n_{k-1}}, \ \dots, \ \exists a_2 \in \{0,1\}^{n_2}, \ \forall a_1 \in \{0,1\}^{n_1} : \sum_{l=1}^{k-1} A_l a_l \not\geq 1 + c.$$

We show that (Even-KLP) is infeasible. Assume, by contradiction, that there is a feasible solution $(y, x_{k-1}, \dots, x_1, s, z_{k-1}, \dots, z_1, z_s)$ of (Even-KLP).

Let $a_{k-1} = \frac{1}{y} x_{k-1}$. Since $x_{k-1} \in \{0, y\}^{n_{k-1}}$, then $a_{k-1} \in \{0,1\}^{n_{k-1}}$. Then, we show that $s = 0$. Let $l \in \{1, \dots, k-2\}$. For even l, the corresponding level whose goal is to minimise s, will choose $x_l = a_l y$ as the assignment that results in $s = 0$ being the only feasible (and hence optimal) for level 2. We know, by assumption, that such a decision exists independently of what the following levels associated with an odd l value choose x_l to be. For odd l, independently of the x_l selected, we know the following levels associated with an even l value will select the decision that lead to $s = 0$. In both cases, The optimal values of the levels are 0 corresponding to $s = 0$. This value of s however violates the linking constraint $s = y$, so the solution cannot be feasible, and we have reached a contradiction. By arbitrariness of the choice of feasible solution, we conclude that (Even-KLP) is infeasible. Hence, the k-level problem (Even-KLP) is not unbounded. □

3.2 Mixed-integer Multilevel Optimization

In this section, we discuss the computational complexity of deciding unboundedness in mixed-integer multilevel optimization. A mixed-integer linear multilevel problem is a linear multilevel problem where some or all of the variables are restricted to take integer values. For each level $l \in \{1, \dots, k\}$ of a k-level problem, we can define the subset I^l of variables at that level which are integer, and add the corresponding constraints to level l:

$$(x_l)_i \in \mathbb{Z} \quad \forall i \in I^l,$$

where x_l denotes the decision variables of level l.

The decision problem of deciding whether a mixed-integer linear k-level problem is unbounded can be stated as:

Unbounded-MI-KLP:
INSTANCE: $f_k, \ldots, f_1$ rational vectors of appropriate dimension, $C^k, \ldots, C^1$ linear polyhedra (defined by rational coefficients), and $I^k, \ldots, I^1$ index subsets of integer variables at each level.
QUESTION: Is the corresponding mixed-integer k-level model unbounded?

Based on the (k)-Alternating Quantified Satisfiability problem ($\mathcal{B}_k \cap \overline{3\text{CNF}}$ or $\mathcal{B}_k \cup 3\text{CNF}$), we show that Unbounded-MI-KLP is a Σ_k^p-hard problem in Theorem 10. In other words, the decision problem of deciding on unboundedness of a mixed-integer multilevel problem is one level higher in the polynomial complexity hierarchy than the decision problem for linear multilevel problem with the same number of levels. This result follows naturally from the previous section, since the reduction problems used can be equivalently reformulated using binary decision variables, instead of enforcing this integrality with the auxiliary variables z and the extra level setting their value.

Theorem 10 *Unbounded-MI-KLP is Σ_k^p-hard.*

Proof Idea The reduction problems in this proofs are direct adaptations of the ones in Theorem 7, Theorem 8 and Theorem 9, where the constraints $x_l \in [0, y]^{n_l}$ and $z_l = \mathbf{0}$ are replaced with the integrality constraint $x_l \in \{0, 1\}^{n_l}$. Similarly, the constraints $s \in [0, y]$ and $z_s = 0$ are replaced with the integrality constraint $s \in \{0, 1\}$. The variable y is removed, and an auxiliary variable r is introduced to create the unboundedness of any feasible instance of the problem. In addition, the lowest level 1, in which the z variables were optimized, is removed. For more details on these reduction problems see Appendix B. □

4 Algorithmic Approaches

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

4.1 LPCC Reformulation

The first approach consists in reformulating our decision problem as a linear problem with complementarity constraints (LPCC). Such problems can be inputted into mixed-integer linear solvers like Gurobi, where complementarity constraints are handled using SOS constraints of type 1. As shown in Theorem 11, the objective value of this LPCC allows us to conclude whether the corresponding bilevel problem is unbounded.

Theorem 11 *The bilevel problem (B) is unbounded if and only if the LPCC (U) has strictly negative optimal value.*

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

where once again $\mathcal{F}_{HPR} \times \mathcal{F}_D = \{(x, y, \lambda) : (B.2),\ (B.4),\ D^\top \lambda = -f,\ \lambda \ge 0\}$*. Moreover, for any feasible solution with strictly negative value exists, the component* (x, y) *provides a feasible point and the component* $(\Delta x, \Delta y)$ *a direction of unboundedness at* (x, y)*.*

Proof According to Theorem 1 and Theorem 2, we can prove this theorem by showing the following equivalence instead: There exists $\omega \in \{1, 2\}^{n_2}$ such that the linear problem (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 $\omega_i^\star = 1$ when $\lambda_i^\star > 0$ and $\omega_i^\star = 2$ when $\lambda_i^\star = 0$. 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 $(\Delta x^\star, \Delta y^\star, \mathbf{0})$ there is a sequence $\{(x^\star, y^\star, \lambda^\star) + k(\Delta x^\star, \Delta y^\star, \mathbf{0})\}_{k\in\mathbb{Z}_0^+}$ 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. □

Note that we can extract further conclusions about the corresponding bilevel problem (B), from the optimization status and optimal value of the problem (U). The problem (U) cannot be unbounded, because of constraint (U.7). When the model (U) is infeasible, so is the bilevel problem (B). We know this because $(\Delta x, \Delta y) = (\mathbf{0}, \mathbf{0})$

is always feasible for (U), so infeasibility of this model reveals that there is no bilevel feasible point (x, y, λ). When the model (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 11 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. In this case, the component (x, y) of optimal solution yield a bilevel feasible point.

4.2 Vertex-enumeration Algorithm

In this section, we present another approach to detect bilevel unboundedness. This approach is a vertex-enumeration algorithm and it is detailed in Algorithm 1. This algorithm is inspired by the observation that, for a fixed dual variable λ, the problem (U) becomes a linear problem. Furthermore, the feasible space of the dual of the lower-level problem

$$\mathcal{F}_{\text{D}} = \{\lambda \geq 0 : D^{\top}\lambda = -f\}$$

only depends on the dual variables λ. Therefore, we can check all vertices of this set $\mathcal{F}_{\text{D}}$, and for each vertex solve a linear problem (step 2) to determine whether there is a corresponding certificate of unboundedness for the bilevel. In other words, we simultaneously search for a bilevel feasible point (x, y), and a direction of unboundedness $(\Delta x, \Delta y)$ which belong to the same polyhedron $\mathcal{P}_\omega$ as the fixed dual vertex λ.

Algorithm 1: Vertex-enumerating algorithm.

1 **for** v_λ *vertex of* $\mathcal{F}_D$ **do**
2   Solve linear model (U'): (U) for $\lambda = v_\lambda$ fixed;
3   **if** *Optimal value of* $(U') < 0$ **then**
4   STOP: Bilevel model (B) is unbounded;
5 CONCLUDE: Bilevel model (B) is bounded (optimal or infeasible);

Note that similarly to the discussion at the end of Section 4.1, we are able to extract further conclusions about the feasibility and optimality of the bilevel problem from Algorithm 1.

Another natural idea would be to enumerate the vertices of the feasible set of the HPR and corresponding extreme rays in search of an unbounded polyhedra $\mathcal{P}_\omega$. Nevertheless, a preliminary computational experience revealed that the enumeration of the dual vertices shows more potential. Hence, we focus solely on Algorithm 1 in this work.

In order to ensure the correctness of Algorithm 1, we present Lemma 12.

Lemma 12 *The bilevel problem (B) is unbounded if and only if there exists λ a vertex of the feasible region of the lower-level dual problem $\mathcal{F}_D$ such that the corresponding (U') has strictly negative optimal value.*

Proof If there exists λ a vertex of the feasible region of the lower-level dual problem $\mathcal{F}_{\text{D}}$ such that the corresponding (U') has strictly negative optimal value, then (U) also has strictly negative optimal value. From Theorem 11, we know that the bilevel problem (B) is unbounded.

If the bilevel problem (B) is unbounded, from Lemma 1 and Theorem 2, 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.

Note that $\mathcal{P}_\omega = \mathcal{P}_\omega^{(x,y)} \times \mathcal{P}_\omega^{\lambda}$, where $\mathcal{P}_\omega^{(x,y)} = \{(x,y) \in \mathcal{F}_{\text{HPR}} : Cx + Dy = b\ \forall i : \omega_i = 1\}$ and $\mathcal{P}_\omega^{\lambda} = \{\lambda \in \mathcal{F}_{\text{D}} : \lambda_i = 0\ \forall i : \omega_i = 2\}$. Hence, since $\mathcal{P}_\omega$ is non-empty, then both $\mathcal{P}_\omega^{(x,y)}$ and $\mathcal{P}_\omega^{\lambda}$ are also non-empty. Since $\mathcal{P}_\omega^{\lambda}$ is non-empty, we know that it has a vertex, because the corresponding constraint matrix has full-row rank, i.e.

$$\text{span}\left\{[D_i^\top]_{i\in\{1,\dots,n_\lambda\}}, [e_i]_{i\in\{1,\dots,n_\lambda\}}\right\} = \mathbb{R}^{n_2},$$

where e_i is the i^{th} unit vector, and n_λ is the number of lower-level dual variables λ. In fact, this property holds valid for any problem in standard form, i.e. with non-negativity constraints. Let $(x,y) \in \mathcal{P}_\omega^{(x,y)} = \{(x,y) \in \mathcal{F}_{\text{HPR}} : Cx + Dy = b\ \forall i : \omega_i = 1\}$, which we know is non-empty. Then $(x,y,\lambda) \in \mathcal{P}_\omega = \mathcal{P}_\omega^{(x,y)} \times \mathcal{P}_\omega^{\lambda}$. Furthermore, since ($\mathrm{P}_\omega$) is a linear problem, we know that $(\Delta x, \Delta y, \Delta\lambda)$ is a direction of unboundedness for (P_ω) at (x,y,λ). Therefore, applying a similar argument to the one in the proof of Theorem 11, we know that $(x,y,\lambda,\Delta x,\Delta y)$ is a feasible solution of problem (U) and that it has strictly negative objective value. Hence, $(x,y,\Delta x,\Delta y)$ is a feasible solution of problem (U') for fixed variables λ, which is a vertex of $\mathcal{F}_{\text{D}}$, and this solution $(x,y,\Delta x,\Delta y)$ has strictly negative objective value. □

The preceding Lemma 12 along with the fact that the feasible set $\mathcal{F}_{\text{D}}$ has a finite number of vertices, lead us to the conclusion that:

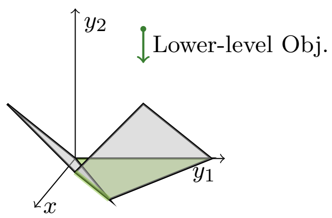
Theorem 13 *Algorithm 1 determines in a finite number of steps whether (B) is unbounded, and if so, it returns a certificate of unboundedness. This certificate consists of a bilevel feasible point and a direction of boundedness at that point.*

4.3 Insights from Illustrative Examples

We illustrate the behaviour of these algorithmic approaches, the LPCC reformulation, and the vertex-enumeration Algorithm 1 on three examples. Example 2 and Example 3 consist of unbounded bilevel problems, and Example 4 is an example of a bounded bilevel with an unbounded HPR.

Example 2 (Book Spine) Consider the unbounded bilevel model below and the corresponding graph, where the bilevel feasible region is coloured green, and the direction is that of improving lower-level objective.

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

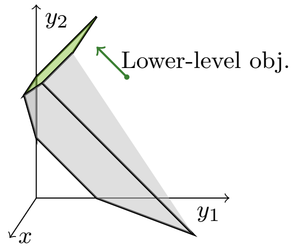


In this example the sequence of points leading to unboundedness of the bilevel lays on the intersection of two facets defined by lower-level constraints, this is along the “book spine”. There is not a single lower-level facet that is unbounded (and bilevel feasible), but rather the intersection of two 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 (see Section 4.4.1 for further details), the vertex-enumeration algorithm only performed one iteration, exploring one vertex of the dual feasible region $\mathcal{F}_{\mathrm{D}}$. The dual vertex found was $(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = (\frac{1}{2}, \frac{1}{2}, 0, 0)$, where λ_3 and λ_4 are the dual variables associated with the non-negativity constraints on y_1 and y_2, respectively. The model (U’) is solved for this dual vertex, and the feasible point and direction of unboundedness are found. Thus, the algorithm concludes correctly that the bilevel problem is unbounded, and that $(1,0,1)$ is a direction of unboundedness at the bilevel feasible point $(1,1,0)$.

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

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

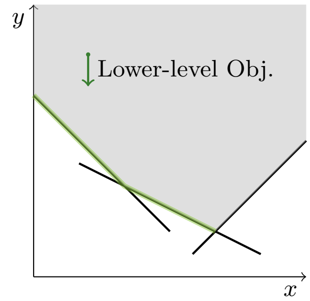


This example is relevant because even though the upper-level variables x are bounded, and the lower-level problem is finite optimal for each feasible value of x, the bilevel is unbounded. This is possible, because for fixed variables x, the lower-level is bounded (with respect to the lower-level objective), but it has an infinite number of optimal solutions that form a sequence of bilevel feasible points with improving 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 (see Section 4.4.1 for further details), the vertex-enumeration algorithm only performed one iteration, exploring one vertex of the dual feasible region $\mathcal{F}_{\mathrm{D}}$. The dual vertex found was $(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = (1,0,0,0)$, where λ_3 and λ_4 are the dual variables associated with the non-negativity constraints on y_1 and y_2, respectively. The model (U’) is solved for this dual vertex, and the feasible point and direction of unboundedness are found. Thus, the algorithm concludes correctly that the bilevel problem is unbounded, and that $(0,1,1)$ is a direction of unboundedness at the bilevel feasible point $(0,0,2)$.

Example 4 (Bounded Bilevel) Consider the bilevel model below and the corresponding graph, where the bilevel feasible region is coloured green, and the direction is that of improving lower-level objective.

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



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 (see Section 4.4.1 for further details), the vertex-enumeration algorithm checks all possible vertices to get to this same conclusion. For example, when it finds the dual vertex $(\lambda_1, \lambda_2, \lambda_3) = (0, 0, 1)$, the corresponding model (U') is infeasible. From constraints (U.3), we have that $y = 0$. By substituting this in the upper-level constraint, we obtain that $x \leq 3$, and in the lower-level constraints, we obtain that $x \geq 6$. These simultaneous restrictions deem the problem (U') infeasible. Alternatively, when the dual vertex $(\lambda_1, \lambda_2, \lambda_3) = (0, 1, 0)$ is found, the corresponding model (U') has optimal value 0. There is a bilevel feasible point $(x, y) = (2, 2)$ that verifies the complementarity constraints with this dual vertex. However, from constraints (U.6), we have that $-\Delta x - \Delta y = 0$, and since both variables Δx and Δy are non-negative, the only solution is $(\Delta x, \Delta y) = (0, 0)$. In other words, there is no direction of unboundedness of the bilevel problem at this dual vertex.

Thus, Algorithm 1 discards both of these dual vertices, and keeps searching. As a matter of fact, since the bilevel is bounded, all dual vertices are discarded either because (a) they do not have a corresponding bilevel feasible solution (x, y), (b) there is no direction of unboundedness at any of the bilevel feasible solution with which the dual vertex matches.

4.4 Computational Comparison

4.4.1 Implementation Details

For our instance set, we considered the linear relaxations of the mixed-integer bilevel problems from the *BOBILib: Bilevel Optimization (Benchmark) Instance Library* [26]. Since all instances had a bounded HPR, we further relaxed the explicit bounds on the decision variables to the standard form of non-negativity constraints, i.e. for all variables v, we defined $v \in [0, +\infty[$. With this procedure we obtained 48 linear bilevel instances whose HPR was unbounded. The names of these instances can be found in the Supplementary Materials.

All computational experiments were conducted on a Dell PowerEdge R740 server running Ubuntu, equipped with four Intel Gold 6234 processors (3.3 GHz, 8 cores/16 threads each) and 1.5TB of local storage. The implementation was done in Python [27], and optimization models were solved with the Gurobi 11.0.1 [28].

For the implementation of the vertex-enumeration procedure in our algorithms, we used the pre-compiled binaries available at [29], which contain the *lrs* reverse search vertex-enumeration algorithm [30]. We impose a two-hour time limit, and a four-thread limit on the *lrs* vertex enumeration, and increase the maximum number of cached dictionaries from 50 to 100. Since solving each optimization problem (U') may take longer than enumerating vertices, some problems (U') may remain unsolved when the time limit is reached. In this case, we continue solving these remaining problems (U') after the vertex enumeration stops. We also impose the same time limit and a limit of four threads on the Gurobi solver when solving the linear problem with complementarity constraints (U).

4.4.2 Results and Discussion

In Table 1, we depict the average of the total computational time (in seconds) to solve instances with both the LPCC approach and the vertex-enumeration Algorithm 1. We present this average per bilevel optimality status, and the total average on the last line. For each of these averages, we also show in the column # *Instances*, the number of instances that were categorized within the time limit.

Table 1 Average total computational time (in seconds) per optimality status.

	LPCC		Vertex-enumeration Algorithm 1	
Bilevel Status	# Instances	CPU Time (s)	# Instances	CPU Time (s)
Unbounded	15	6.396	9	5241.181
Finite Optimal	25	22.629	11	1270.638
Infeasible	8	0.121	8	0.377
Total	48	13.805	28	6882.173

We observe that the vertex-enumeration Algorithm 1 has a higher computational time in all categories. While this difference is significant for unbounded and finite optimal instances, Algorithm 1 is quick at detecting infeasible instances. This is due to the fact that this infeasibility stems from an unbounded lower-level problem, or equivalently an infeasible dual lower-level problem.

Furthermore, due to the time limit imposed on the *lrs* vertex-enumeration, Algorithm 1 was only able to arrive at a definitive conclusion about whether the bilevel problem was unbounded for 28 of the 48 instances. In Table 2, we further explore this theme, and consider the number of instances with each optimality status (including an inconclusive one) for which the *lrs* algorithm reached the time limit and not. Note that if the *lrs* algorithm does not time out, a proper optimality status will always be found and an inconclusive status is not possible. Similarly, if the *lrs* algorithm times out, we will not be able to conclude that the instance is finite optimal nor infeasible, as we would have to explore all dual vertices to reach that conclusion. In case, we were not able to decide whether the bilevel instance is unbounded nor feasible, an *Inconclusive* status is assigned, and if we were not able to decide whether the bilevel instance is unbounded, but we did find a feasible solution, an *Inconclusive Feasible* status is assigned.

Table 2 Number of instances with each optimality status from the dual enumeration algorithm (out of 48).

	lrs Timed Out?	
Bilevel Status	Yes	No
Unbounded	5	4
Finite Optimal	-	11
Infeasible	-	8
Inconclusive	15	-
Inconclusive Feasible	5	-
Total	25	23

We can observe that the *lrs* algorithm reached its two-hour time limit on 25 of the instances, but in five of those instances it was still able to conclude the bilevel was unbounded, since the dual vertex that allows this had already been found before the time out. Out of those 25, it could discard infeasibility in five instances, but nothing was concluded in the remaining 15.

While in the LPCC approach most of the computational time is spent solving the model, in Algorithm 1 there are two tasks where the algorithm spends most of its time. The first is naturally running the *lrs* vertex-enumeration algorithm, which takes on average 4129.761 seconds, and the second is building and solving the linear problems at each vertex found, with an average of 3087.721 seconds spend on building and 1597.400 seconds on solving these problems. Note that each instance solved, on average, 3542190.3 of these linear problems corresponding to the number of vertices evaluated until either one that resulted in unboundedness was found or all were explored. Our implementation performs this evaluation of vertices dynamically as they are found and outputted by the *lrs* algorithm, and 63% of the evaluated vertices were processed while the *lrs* was still running.

In conclusion, these results suggest that directly solving a theoretically intractable problem can be more effective than solving a potentially very large number of polynomially solvable subproblems. This supports the idea that solving of the LPCC gains by being driven by leader's objective.

5 Conclusion

We presented results aimed at dealing with the often-overlook topic of unboundedness in bilevel and multilevel optimization. In Table 3, we summarise the computational complexity results derived in this work. In general, we show that deciding unboundedness of an optimistic k-level problem is Σ^p_{k-1}-hard for linear problems and Σ^p_k-hard for mixed-integer problems. In the bilevel case, we extend the hardness result for pessimistic formulations by showing that deciding on unboundedness in these problems is also NP-hard.

Future research could focus on deriving the computational complexity of deciding unboundedness of mixed-integer pessimistic multilevel problems, or of multi-follower

Table 3 Overview of computational complexity of deciding unboundedness.

	Bilevel		Multilevel (k levels)
	Optimistic	Pessimistic	Optimistic
Linear	NP-complete	NP-hard	Σ^p_{k-1}-hard
Mixed-integer	Σ^p_2-hard		Σ^p_k-hard

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 linear optimization problems. However, if the bilevel problem (B) is bounded (and its HPR unbounded), we must enumerate all vertices of the lower-level dual feasible region. 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 an incumbent solution. Furthermore, developing heuristics to prioritize the enumeration of vertices of the dual feasible space that correspond to primal lower-level faces which are unbounded for the HPR may enhance the algorithm's efficiency in proving unboundedness.

Finally, this work demonstrates that more attention should be paid to ensure unboundedness is accounted for and dealt with in bilevel and multilevel optimization. This can be achieved by ensuring that deciding on unboundedness and returning a certificate of unboundedness, if one exists, become integral practices when developing multilevel algorithmic approaches. In addition, designing a diverse dataset of bilevel problems with a) unbounded bilevel instances and b) bounded (optimal or infeasible) bilevel instances whose corresponding HPR is unbounded would also be desirable, as these are scarce in existent datasets [26, 31, 32].

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Appendix A Strong NP-hardness with Linking Constraints

In this section, we show that UNBOUNDED-BLP is strongly NP-hard for problems with linking constraints. Naturally, the hardness result for problems without linking constraints in Section 2.2.2 is stronger. Nevertheless, the ideas used for the reduction proof with linking constraints are useful for building intuition for the multilevel linear case in Section 3.1. This is the main reason why, in this appendix, we introduce the hardness proof for deciding on unboundedness of bilevel problems with linking constraints.

Theorem 14 *UNBOUNDED-BLP with linking constraints is strongly NP-complete.*

Proof From Lemma 1 and Theorem 2, 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.

$$
\begin{aligned}
\max_{x,y,z} \quad & y && \text{(B')}\\
\text{s.t.} \quad & A_{\text{S}} x \geq (1+c_{\text{S}})y, \\
& 0 \leq x_i \leq y \quad \forall i \in \{1,\dots,n\}, \\
& y \geq 1, \\
& z = \mathbf{0}, \\
& z \in \arg\max_{\bar{z}} \left\{ \sum_{i=1}^{n} \bar{z}_i : \bar{z}_i \leq x_i;\ \ \bar{z}_i \leq y - x_i \ \forall i \in \{1,\dots,n\} \right\}.
\end{aligned}
$$

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 $(x^*, y^*, z^*) = (a, 1, \mathbf{0})$, and a direction of unboundedness with $(\Delta x, \Delta y, \Delta z) = (a, 1, \mathbf{0})$. 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 $z = \mathbf{0}$. Hence, (B') is not unbounded. □

Appendix B Complete Proof of Theorem 10

In this section, we present a complete proof of Theorem 10 where we explicitly present the reduction problems considered.

Proof For $k = 2$, the mixed-integer bilevel problem used in the reduction is:

$$
\begin{aligned}
\max_{r, x_2, x_1, s} \quad & r \\
\text{s.t.} \quad & r \in \mathbb{R}, \\
& x_2 \in \{0,1\}^{n_2}, \\
& s = 0, \\
& (x_1, s) \in \arg\max_{x_1, s} \quad s \\
& \qquad\qquad \text{s.t.} \quad \sum_{i=1}^{2} A_i x_i \geq s + c, \\
& \qquad\qquad\qquad x_1 \in \{0,1\}^{n_1}, \\
& \qquad\qquad\qquad s \in \{0,1\},
\end{aligned}
$$

The proof showing that this problem reduces to $\mathcal{B}_2 \cap \overline{\text{3CNF}}$ is similar to that of Theorem 7 for trilevel linear problems. This shows that if $\mathcal{B}_2 \cap \overline{\text{3CNF}}$ is a YES instance, the reduction problem is unbounded, and if it is a NO instance, the reduction problem is infeasible (i.e. not unbounded).

In general, for a multilevel problem, we separate the odd and even cases. For k even, we adapt the reduction problem in Theorem 8 as:

$$\begin{aligned}
\max_{r,x,s,z} \quad & r \\
\text{s.t.} \quad & r \in \mathbb{R}, \\
& x_k \in \{0,1\}^{n_k}, \\
& s = 0, \\
& \qquad \vdots \\
l \text{ odd: } & (x^{(l)}, s) \in \arg\max_{x^{(l)},s} \left\{ s : x_l \in \{0,1\}^{n_l}, (x^{(l-1)}, s) \in \Phi^{l-1} \right\}, \\
l \text{ even: } & (x^{(l)}, s) \in \arg\min_{x^{(l)}} \left\{ s : x_l \in \{0,1\}^{n_l}, (x^{(l-1)}, s) \in \Phi^{l-1} \right\}, \\
& \qquad \vdots \\
& (x_1, s) \in \arg\max_{x_1,s} \quad s \\
& \qquad\qquad \text{s.t.} \quad \sum_{i=1}^{k-1} A_i x_i \geq s + c, \\
& \qquad\qquad\qquad x_1 \in \{0,1\}^{n_1}, \\
& \qquad\qquad\qquad s \in \{0,1\},
\end{aligned}$$

The proof showing that this mixed-integer k-level problem reduces to $\mathcal{B}_k \cap \overline{3\text{CNF}}$ is similar to that of Theorem 8. It shows that if $\mathcal{B}_k \cap \overline{3\text{CNF}}$ is a YES instance, the reduction problem is unbounded, and if it is a NO instance, the reduction problem is infeasible (i.e. not unbounded).

For k odd, we adapt the reduction problem in Theorem 9 as:

$$\begin{aligned}
\max_{r,x,s,z} \quad & r \\
\text{s.t.} \quad & r \in \mathbb{R}, \\
& x_k \in \{0,1\}^{n_k}, \\
& s = y, \\
& \qquad \vdots \\
l \text{ odd: } & (x^{(l)}, s) \in \arg\max_{x^{(l)},s} \left\{ s : x_l \in \{0,1\}^{n_l}, (x^{(l-1)}, s) \in \Phi^{l-1} \right\}, \\
l \text{ even: } & (x^{(l)}, s) \in \arg\min_{x^{(l)}} \left\{ s : x_l \in \{0,1\}^{n_l}, (x^{(l-1)}, s) \in \Phi^{l-1} \right\}, \\
& \qquad \vdots \\
& (x_1, s) \in \arg\max_{x_1,s} \quad s \\
& \qquad\qquad \text{s.t.} \quad \sum_{i=1}^{k-1} A_i x_i \geq s + c, \\
& \qquad\qquad\qquad x_1 \in \{0,1\}^{n_1}, \\
& \qquad\qquad\qquad s \in \{0,1\},
\end{aligned}$$

The proof showing that this mixed-integer k-level problem reduces to $\mathcal{B}_k \cup 3\text{CNF}$ is similar to that of Theorem 9. It shows that if $\mathcal{B}_k \cup 3\text{CNF}$ is a YES instance, the reduction problem is unbounded, and if it is a NO instance, the reduction problem is infeasible (i.e. not unbounded). □

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