On Linear Bilevel Optimization Problems with Complementarity-Constrained Lower Levels

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Abstract. We consider a novel class of linear bilevel optimization models with a lower level that is a linear program with complementarity constraints (LPCC). We present different single-level reformulations depending on whether the linear complementarity problem (LCP) as part of the lower-level constraint set depends on the upper-level decisions or not as well as on whether the LCP matrix is positive definite or positive semidefinite. Moreover, we illustrate the connection to linear trilevel models that can be reduced to bilevel problems with LPCC lower levels having positive (semi)definite matrices. Finally, we provide two generic and illustrative bilevel models from the fields of transportation and energy to show the practical relevance of the newly introduced class of bilevel problems and show related theoretical results.

1. Introduction

Bilevel optimization problems have received increasing attention over the last years. One specific reason is their capability of representing hierarchical decision making processes that are of tremendous importance for modeling many applications; see, e.g., Daxhelet and Smeers (2007), Grimm et al. (2019), Hu and Ralph (2007), and Kleinert and Schmidt (2019) for applications in energy markets, Caprara et al. (2016) and DeNegre (2011) for critical infrastructure defense, or Labbé and Violin (2013) for bilevel pricing models with applications in revenue management. However, it is well-known that bilevel optimization problems are strongly NP-hard even for their easiest instantiation with linear lower- and upper-level problems (Hansen et al. 1992; Jeroslow 1985).

Nevertheless, bilevel modeling is frequently used. Although many solution techniques such as branch-and-bound (Moore and Bard 1990), branch-and-cut (DeNegre and Ralphs 2009; Fischetti et al. 2017, 2018; Tahernejad et al. 2020), or penalty methods (Kleinert and Schmidt 2020; White and Anandalingam 1993) have been developed over the last few years, the approach most often used in practice still relies on the reformulation of the bilevel problem to a single-level problem by exploiting suitable optimality conditions of the lower-level problem such as the Karush–Kuhn–Tucker (KKT) conditions or the strong duality theorem. However, these approaches are only applicable if such optimality conditions are available, which is, in general, only the case for convex lower-level problems satisfying a constraint qualification. The latter type of lower-level problems can be considered as the easiest one to be tackled in the context of bilevel optimization. Hence, the algorithmic striving of the last years was therefore characterized by the development of new procedures for more and more complex lower levels such as nonconvex but continuous (Mitsos et al. 2008) as well as purely or mixed-integer lower levels (DeNegre and Ralphs 2009; Fischetti et al. 2017, 2018).

The contribution of this paper is in line with the above-mentioned references. We consider a novel class of bilevel problems in which the lower-level problem is challenging itself because it is a linear program with complementarity constraints (LPCC; see, e.g., Hu

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et al. (2008, 2012) and Yu et al. (2019)). To the best of our knowledge, this class of problems has not been studied before in the literature. However, in contrast to the more recent literature dealing with hard lower-level problems that typically has a strong algorithmic focus, we consider reformulations of the novel type of lower-level problems to obtain single-level reformulations that can be dealt with in practice. To this end, we exploit the classic theory of linear complementarity problems (LCPs); see, e.g., the seminal textbook by Cottle et al. (2009). Whereas for "usual" convex lower levels, optimality conditions are the most prominent tool to obtain single-level reformulations, it turns out that the structural insights on the LCP's solution set are key for LPCC lower levels. Thus, the main contribution of this paper is the combination of well-known structural properties of LCPs with positive (semi)definite matrices with classic reformulations of bilevel problems with linear lower levels using their optimality conditions. Let us further highlight the very challenging character of the considered class of bilevel problems by discussing approaches from the literature that can deal with nonlinear and nonconvex lower-level problems as well. One well-known approach is the branch-and-sandwich method that can also handle nonlinear and nonconvex lower-level problems; see, e.g., Kleniati and Adjiman (2014a) and Kleniati and Adjiman (2014b). However, this approach requires finite bounds on all variables in the lower level, which is not the case for LCP variables, and also requires a constraint qualification (CQ) for the lower-level problem, which is never satisfied for LCP constraints; see, e.g., Ye and Zhu (1995). Moreover, the value-function based approach presented in Lozano and Smith (2017) can also tackle nonlinear and nonconvex lower-level problems but requires, e.g., that all linking variables are integer. Thus, a completely different setting is considered compared to what we study in this paper. Further, the BiOpt Toolbox solvers also require a CQ to be satisfied for the lower-level problem, which is never the case for LCPs in the lower level.[1] To sum up, we are not aware of any algorithmic approaches in the literature on nonlinear bilevel optimization that can solve the class of problems considered in this paper.

After stating the considered class of problems in Section 2, we then distinguish between whether the lower-level LCP constraints are independent (Section 3) or dependent (Section 4) on the upper-level decisions. Furthermore, we always split the analysis along the definiteness of the LCP matrix—with a special emphasis on positive definite or positive semidefinite matrices. Practically useful single-level reformulations are derived for the case of a positive definite or a positive semidefinite matrix, whereas the case of lower-level LPCCs with indefinite LCP matrix already contains the case of (mixed-)integer lower-level problems, which is out of the scope of this paper. The connection to linear or quadratic trilevel problems is discussed in Section 5 but differs from other trilevel approaches, e.g., in infrastructure modeling; see Gu et al. (2019) and Jin and Ryan (2013). Finally, we provide two generic and illustrative bilevel problems with LPCC lower levels from transportation (the spatial price equilibrium problem) and energy (a Nash–Cournot oligopoly for power production) in Section 6 to illustrate the practical relevance of the considered class of bilevel problems and prove related results for those two classes of problems. These two generic examples for the lower-level LCP are well-studied problems. However, embedding them in the computationally attractive way we did, leading to an overall trilevel equilibrium model, is novel as are the theorems relating to the positive semi-definiteness of the resulting complementarity problems' matrices. The paper closes with some concluding remarks in Section 7.

[1]See `https://biopt.github.io/solvers/` and the papers referred to in the technical report Zhou and Zemkoho (n.d.).

2. Problem Statement

We consider the following bilevel optimization problem with a lower level that is given as an LPCC:

$$\min_{x,y} \quad c^\top x + d^\top y \tag{1a}$$
$$\text{s.t.} \quad Ax + By \geq a, \tag{1b}$$
$$y \text{ solves } \mathrm{LPCC}(x), \tag{1c}$$

where $\mathrm{LPCC}(x)$ denotes the lower-level problem. Here, $c \in \mathbb{R}^{n_x}$, $x \in \mathbb{R}^{n_x}$, $d \in \mathbb{R}^{n_y}$, $y \in \mathbb{R}^{n_y}$, $A \in \mathbb{R}^{m_u \times n_x}$, $B \in \mathbb{R}^{m_u \times n_y}$, and $a \in \mathbb{R}^{m_u}$. As it is indicated in (1), the problem considered is the optimistic bilevel problem in which, in case of multiple solutions of the lower-level problem, the lower-level decision aligns with the upper-level objective.

The LPCC in the lower level is given by

$$\min_{y} \quad e^\top y \tag{2a}$$
$$\text{s.t.} \quad Cx + Dy \geq b, \tag{2b}$$
$$0 \leq y \perp q + Nx + My \geq 0, \tag{2c}$$

i.e., the lower-level constraints contain a linear complementarity problem (LCP) that is parameterized by the upper-level's variables x via the term Nx. Here and in what follows, we use the standard $\perp$-notation

$$0 \leq a \perp b \geq 0 \iff a, b \geq 0, \; a^\top b = 0$$

for vectors a, b. In what follows, we denote by $\mathrm{LCP}(q, M)$ the LCP with vector q and matrix M, i.e., the problem $0 \leq y \perp q + My \geq 0$. Finally, $e \in \mathbb{R}^{n_y}$, $C \in \mathbb{R}^{m_\ell \times n_x}$, $D \in \mathbb{R}^{m_\ell \times n_y}$, and $b \in \mathbb{R}^{m_\ell}$ holds and the LCP data is given by $q \in \mathbb{R}^{n_y}$, $M \in \mathbb{R}^{n_y \times n_y}$, and $N \in \mathbb{R}^{n_y \times n_x}$. We refer to Li and Ierapetritou (2010) and the references therein for a discussion of general parametric LCPs.

The above formulations are quite general and thus admit many interesting applications. As will be shown below, they can be solved rather effectively and this gives promise to being able to apply such a modeling approach for applications—two classes of which we detail in Section 6. In particular, we focus on two trilevel infrastructure problems that have a regulator (federal or regional) at the top level, a network operator at the middle level, and network users at the bottom level. The first one (Section 6.1) takes the classic spatial price equilibrium problem (Gabriel et al. 2012) in transportation as the bottom level but expressed via the complementarity constraints of the LPCC lower level. The second application (Section 6.2) is on power markets where the associated complementarity problem is a Nash–Cournot power production oligopoly (Gabriel et al. 2012). We prove theorems attesting to the positive semi-definiteness of the LCPs associated to these two representative applications as a proof of concept and confirmation to the novel approach which we detail in Sections 3–5.

3. The Case of x-Independent Lower-Level LPCCs

We first assume that the LCP constraints of the lower level do not depend on the upper-level decision x, i.e., the lower level is given by

$$\min_{y} \quad e^\top y \tag{3a}$$
$$\text{s.t.} \quad Cx + Dy \geq b, \tag{3b}$$
$$0 \leq y \perp q + My \geq 0. \tag{3c}$$

This can be seen as the special case of the general lower level (2) with $N = 0$.

Remark 1. *If M is allowed to be indefinite, this setting already includes linear bilevel optimization problems with binary lower-level variables y_i via*

$$0 \le y_i \perp 1 - y_i \ge 0 \iff y_i \in \{0, 1\}.$$

3.1. **Positive Definite M.** Next, we consider the much easier case of M being positive definite. In this case, the LCP(q, M) in the lower-level constraints is solvable and has a unique solution for every $q \in \mathbb{R}^{n_y}$; see, e.g., Theorem 3.1.6 in Cottle et al. (2009). We denote this uniquely determined solution by y^* (which, of course, depends on q and M). Thus, we can re-write the lower-level problem as the feasibility problem $Cx \ge b - Dy^*$, having the corresponding objective function value $e^\top y^*$. This means, there is no optimization problem left to be solved in the lower level and Problem (1) is equivalent to

$$\min_x \quad c^\top x + d^\top y^* \tag{4a}$$

$$\text{s.t.} \quad Ax \ge a - By^*, \tag{4b}$$

$$Cx \ge b - Dy^*. \tag{4c}$$

Note that y^* can be efficiently computed (i.e., in polynomial time; see, e.g., Ye and Tse (1989)) by solving the strictly convex quadratic problem (QP)

$$\min_y \quad y^\top (q + My) \quad \text{s.t.} \quad y \ge 0, \ q + My \ge 0, \tag{5}$$

which has an optimal objective function value of 0 in this case. After solving this problem (to obtain y^*), Problem (4) is a simple linear program (LP) that can also be solved efficiently. Thus, we have shown the following result.

Theorem 2. *The bilevel optimization problem* (1) *with lower level* (3) *and M positive definite can be solved in polynomial time. More specifically, we need to solve a strictly convex QP and an LP.*

The key mathematical property to obtain the results so far is the uniqueness of the LCP's solution, which is guaranteed since the LCP's matrix is positive definite. Note that the uniqueness of the LCP's solution holds in general for P matrices, i.e., for square matrices for which all principal minors are positive; see, e.g., Cottle et al. (2009). Hence, the results in this section carry over to P matrices as well. However, the QP (5) does not need to be strictly convex anymore in the case of P matrices that are not positive definite.

3.2. **Positive Semidefinite M.** We now turn to the case that M is positive semidefinite. If we assume that the LCP(q, M) is feasible[2], it is also solvable (see Theorem 3.1.2 in Cottle et al. (2009)) and a solution can again be computed by solving the QP (5), which is not strictly convex but still convex. Let $\bar{y}$ be a solution of this convex QP. Note that $\bar{y}$ may not be uniquely determined because M is not positive definite. However, the set of all solutions is polyhedral and given by

$$\mathcal{P} = \{y \in \mathbb{R}^{n_y}_{\ge 0} : q + My \ge 0, \ q^\top (y - \bar{y}) = 0, \ (M + M^\top)(y - \bar{y}) = 0\};$$

see, e.g., Theorem 3.1.7 in Cottle et al. (2009). Note that M does not need to be symmetric in this case. If it is symmetric, the last condition simplifies to $M(y - \bar{y}) = 0$. As a consequence of the polyhedral representation of the LCP's solution set, the lower level can be re-written as

$$\begin{aligned} \min_y \quad & e^\top y \\ \text{s.t.} \quad & Cx + Dy \ge b, \\ & q + My \ge 0, \ y \ge 0, \\ & q^\top (y - \bar{y}) = 0, \ (M + M^\top)(y - \bar{y}) = 0. \end{aligned}$$

[2]Note that if the LCP(q, M) is not feasible, neither is the lower-level problem.

This is a parameterized LP with parameters x and $\bar{y}$. Since all constraints of this problem are linear, no other constraint qualification is required and the KKT conditions

$$\begin{aligned} e - D^\top\alpha - M^\top\beta - \gamma - \delta q - (M + M^\top)\varepsilon = 0, \\ Cx + Dy \geq b,\ q + My \geq 0,\ y \geq 0, \\ q^\top(y - \bar{y}) = 0,\ (M + M^\top)(y - \bar{y}) = 0, \\ \alpha^\top(Cx + Dy - b) = 0,\ \beta^\top(q + My) = 0,\ \gamma^\top y = 0, \\ \alpha, \beta, \gamma \geq 0 \end{aligned}$$

are both necessary and sufficient. Here, α, β, γ, δ, and ε are the corresponding dual variables. Using these KKT conditions, we see that Problem (1) is equivalent to

$$\begin{aligned} \min_{x,y,\alpha,\beta,\gamma,\delta,\varepsilon} \quad & c^\top x + d^\top y \\ \text{s.t.} \quad & Ax + By \geq a, \\ & e - D^\top\alpha - M^\top\beta - \gamma - \delta q - (M + M^\top)\varepsilon = 0, \\ & Cx + Dy \geq b,\ q + My \geq 0,\ y \geq 0, \\ & q^\top(y - \bar{y}) = 0,\ (M + M^\top)(y - \bar{y}) = 0, \\ & \alpha^\top(Cx + Dy - b) = 0,\ \beta^\top(q + My) = 0,\ \gamma^\top y = 0, \\ & \alpha, \beta, \gamma \geq 0. \end{aligned}$$

All constraints except for $Ax + By \geq a$ can be re-written as the $(x, \bar{y})$-parameterized mixed LCP (MLCP) of the form

$$G(z^1, z^2; \bar{y}) = 0, \quad 0 \leq z^2 \perp F(z^1, z^2; x) \geq 0,$$

with $z^1 = (\delta, \varepsilon^\top)^\top$, $z^2 = (\beta^\top, y^\top, \alpha^\top)^\top$, and affine-linear functions

$$G(z^1, z^2; \bar{y}) = \begin{pmatrix} -q^\top\bar{y} \\ -(M + M^\top)\bar{y} \end{pmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \delta \\ \varepsilon \end{pmatrix} + \begin{bmatrix} 0 & q^\top & 0 \\ 0 & M + M^\top & 0 \end{bmatrix} \begin{pmatrix} \beta \\ y \\ \alpha \end{pmatrix},$$

$$F(z^1, z^2; x) = \begin{pmatrix} q \\ e \\ Cx - b \end{pmatrix} + \begin{bmatrix} 0 & 0 \\ -q & -(M + M^\top) \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \delta \\ \varepsilon \end{pmatrix} + \begin{bmatrix} 0 & M & 0 \\ -M^\top & 0 & -D^\top \\ 0 & D & 0 \end{bmatrix} \begin{pmatrix} \beta \\ y \\ \alpha \end{pmatrix}.$$

Since the matrix in G corresponding to the free variables z^1 is the zero matrix and, thus, not invertible, this mixed LCP cannot be re-written further to obtain an equivalent LCP. Hence, we have shown the following result.

Theorem 3. *Consider the bilevel optimization problem (1) with the lower-level LPCC (3). If M is positive semidefinite and if the LCP in the lower-level constraints is feasible, the bilevel problem is equivalent to a linear program with additional MLCP constraints.*

Remark 4. *The last theorem also shows that, in the considered setting, having LCP constraints in the lower level of a bilevel problem leads to a problem that seems to be, from the point of view of complexity theory, comparably hard as LP-LP bilevel problems, since the latter can also be solved as single-level LPs with additional MLCP constraints.*

4. The Case of x-Dependent Lower-Level LPCCs

We now face a lower-level problem that is constrained by the x-parameterized LCP

$$0 \leq y \perp q + Nx + My \geq 0$$

as stated in (2). From the point of view of the lower-level problem, x is a given parameter and, hence, $q(x) = q + Nx$ is a given vector.

4.1. **Positive Definite** M**.** Let us again first consider the easiest case in which M is positive definite. Under this assumption, as argued in Section 3, the lower-level LCP($q+Nx, M$) has a unique solution $y^* = y^*(q(x)) = y^*(q+Nx)$ for every $q(x) = q + Nx$, i.e., in particular, for any upper-level decision x. Note that in contrast to Section 3.1, this solution is not independent of the upper-level decision anymore.

Nevertheless, the uniqueness of the LCP's solution allows us to rewrite the bilevel problem as a single-level problem consisting of the upper- and lower-level constraints as well as the upper-level objective function; see Section 3.1. Thus, we have shown the following theorem.

Theorem 5. *The bilevel optimization problem* (1) *with lower level* (2) *and M positive definite is equivalent to the single-level reformulation*

$$\begin{aligned} \min_{x,y,\beta} \quad & c^\top x + d^\top y \\ \text{s.t.} \quad & Ax + By \geq a, \; Cx + Dy \geq b, \\ & 0 \leq y \perp q + Nx + My \geq 0. \end{aligned}$$

This is an LP with additional LCP constraints.

Note that the last theorem states that the bilevel optimization problem (1) with lower level (2) and M positive definite belongs to the same problem class (LPCC) as its lower-level problem. This is different from the results in Section 3.1, since we cannot pre-compute the solution y^* here due to the dependence of y^* on x.

4.2. **Positive Semidefinite** M**.** Now assume that M is positive semidefinite and that we have a solution $\bar{y} = \bar{y}(q(x)) = \bar{y}(q+Nx)$ of the LCP($q+Nx, M$). In contrast to the positive definite case, solvability of the LCP in the lower level is not guaranteed for all vectors $q+Nx$. Instead, we know that the LCP is solvable if it is feasible. Since no x will be chosen that leads to an infeasible lower-level problem, we thus have to make the assumption that there exists at least one feasible x for which the lower-level LCP ($q + Nx, M$) is feasible. We can use the same characterization of the LCP's solution set as in Section 3 and obtain

$$\begin{aligned} \mathcal{P} = \mathcal{P}(x) = \{y \in \mathbb{R}^{n_y}_{\geq 0} : q + Nx + My \geq 0, \; (q+Nx)^\top (y - \bar{y}(q+Nx)) = 0, \\ (M + M^\top)(y - \bar{y}(q+Nx)) = 0\}. \end{aligned}$$

Hence, the lower-level problem can be re-written as

$$\min_{y \geq 0} \quad e^\top y, \tag{6a}$$
$$\text{s.t.} \quad Cx + Dy \geq b, \tag{6b}$$
$$q + Nx + My \geq 0, \tag{6c}$$
$$(q+Nx)^\top (y - \bar{y}(q+Nx)) = 0, \tag{6d}$$
$$(M + M^\top)(y - \bar{y}(q+Nx)) = 0. \tag{6e}$$

Theorem 6. *Let M be a positive semidefinite matrix. Then, (x^*, y^*) is an optimal solution of Problem* (1) *with lower level* (2) *if and only if $(x^*, y^*, \bar{y}^*)$ is an optimal solution of the problem*

$$\min_{x,y,\bar{y}} \quad c^\top x + d^\top y \tag{7a}$$
$$\text{s.t.} \quad Ax + By \geq a, \tag{7b}$$
$$\bar{y} \in \operatorname*{arg\,min}_{y' \geq 0} \{y'^\top (q + Nx + My') : q + Nx + My' \geq 0\}, \tag{7c}$$
$$\begin{aligned} y \in \operatorname*{arg\,min}_{\hat{y} \geq 0} \Big\{ e^\top \hat{y} : q + Nx + M\hat{y} \geq 0, \; (q+Nx)^\top (\hat{y} - \bar{y}) = 0, \\ (M + M^\top)(\hat{y} - \bar{y}) = 0, \; Cx + D\hat{y} \geq b \Big\}. \end{aligned} \tag{7d}$$

with $(\bar{y}^*)^\top(q + Nx^* + M\bar{y}^*) = 0$.

Proof. Note first that the objective functions of both problems are the same. Hence, we only need to check that for every feasible point of Problem (1) there is a feasible point of Problem (7) and vice versa.

Let us first suppose that (x^*, y^*) is a feasible solution of Problem (1) with lower level (2) and let $\bar{y}^* = \bar{y}(q(x^*))$ be a solution of the LCP$(q(x^*), M)$. We now prove that $(x^*, y^*, \bar{y}^*)$ is a feasible solution of Problem (7). Constraint (7b) is clearly satisfied since it is also part of Problem (1). By definition of $\bar{y}^*$, (7c) and $(\bar{y}^*)^\top(q + Nx^* + M\bar{y}^*) = 0$ are also fulfilled. We already showed that Problem (2) is equivalent to Problem (6) for M being positive semidefinite. Then, $(x^*, y^*, \bar{y}^*)$ solves (6) and, hence, it also fulfills (7d).

Let us assume now that $(x^*, y^*, \bar{y}^*)$ is feasible for Problem (7). We show that (x^*, y^*) is feasible for Problem (1) with lower level (2). Constraint (1b) is again clearly satisfied by (x^*, y^*). Moreover, $\bar{y}^*$ is a solution of LCP$(q(x^*), M)$ due to Constraint (7c) and the condition $(\bar{y}^*)^\top(q + Nx^* + M\bar{y}^*) = 0$. In addition, y^* is optimal for (6) for $(x^*, \bar{y}^*)$ due to Constraint (7d). As discussed before, Problem (2) is equivalent to Problem (6) for $\bar{y}^* = \bar{y}(x^*)$ and, thus, (x^*, y^*) is feasible for (2). □

For any given x, the two nested optimization problems in (7) are a convex QP and an LP, respectively. Hence, the KKT conditions of both problems are necessary and sufficient and the two inner problems can be replaced by their KKT conditions, leading to the single-level reformulation

$$
\begin{aligned}
\min_{x,y,\bar{y},\beta,\gamma,\delta,\zeta,\eta} \quad & c^\top x + d^\top y \\
\text{s.t.} \quad & Ax + By \geq a, \\
& 0 \leq \bar{y} \perp q + Nx + 2My - M^\top \beta \geq 0, \\
& 0 \leq \beta \perp q + Nx + M\bar{y} \geq 0, \\
& 0 \leq y \perp e - D^\top \gamma - M^\top \delta - \zeta^\top (q + Nx) - (M + M^\top)^\top \eta \geq 0, \\
& 0 \leq \delta \perp (q + Nx) + My \geq 0, \\
& (q + Nx)^\top (y - \bar{y}) = 0, \ (M + M^\top)(y - \bar{y}) = 0, \\
& 0 \leq \gamma \perp Cx + Dy - b \geq 0.
\end{aligned}
$$

Remark 7. *What we have seen so far is that, if the matrix of the lower-level LCP is positive semidefinite, the problem can be reformulated as an mathematical program with complementarity constraints (MPCC). In contrast to the results from the last section, this MPCC is not linear anymore due to the nonlinear products* $\zeta^\top Nx$ *as well as the products* $(Nx)^\top y$ *and* $(Nx)^\top \bar{y}$.

5. Application to Trilevel Models

We now study under which assumptions LP-LP-LP trilevel models can be re-written as a single-level problem by using the theoretical results obtained in the previous sections. To this end, we consider LP-LP-LP trilevel models defined by the following three levels:

- Level 1: $\min_{x \geq 0, y, z} \{c_1^\top x + d_1^\top y + e_1^\top z \colon A_1 x + B_1 y + C_1 z \geq a_1\}$,
- Level 2: $\min_{y \geq 0, z} \{d_2^\top y + e_2^\top z \colon A_2 x + B_2 y + C_2 z \geq a_2\}$,
- Level 3: $\min_{z \geq 0} \{e_3^\top z \colon A_3 x + B_3 y + C_3 z \geq a_3\}$.

In particular, we study under which assumptions these trilevel models correspond to a bilevel problem with an LPCC in the lower level that has a positive (semi)definite matrix.

The KKT conditions of the third level are given by

$$0 \leq z \perp e_3 - C_3^\top \lambda \geq 0, \quad 0 \leq \lambda \perp A_3 x + B_3 y + C_3 z - a_3 \geq 0.$$

If we now replace the third level by these necessary and sufficient optimality conditions, the second level translates to

$$\begin{aligned}\min_{y\geq 0,z,\lambda} \quad & d_2^\top y + e_2^\top z\\ \text{s.t.} \quad & A_2x + B_2y + C_2z \geq a_2,\\ & 0 \leq z \perp e_3 - C_3^\top \lambda \geq 0,\\ & 0 \leq \lambda \perp A_3x + B_3y + C_3z - a_3 \geq 0.\end{aligned}$$

Using the notation $C = A_2$, $D = [B_2, C_2, 0]$, and $b = a_2$, as well as

$$\tilde{y} = \begin{pmatrix} y\\ z\\ \lambda\end{pmatrix}, \quad \tilde{e} = \begin{pmatrix} d_2\\ e_2\\ 0\end{pmatrix}, \quad q = \begin{pmatrix} 0\\ e_3\\ -a_3\end{pmatrix}, \quad N = \begin{bmatrix} 0\\ 0\\ A_3\end{bmatrix}, \quad M = \begin{bmatrix} 0 & 0 & 0\\ 0 & 0 & -C_3^\top\\ B_3 & C_3 & 0\end{bmatrix},$$

we can recast the reformulated second-level problem as

$$\begin{aligned}\min_{\tilde{y}} \quad & \tilde{e}^\top \tilde{y}\\ \text{s.t.} \quad & Cx + D\tilde{y} \geq b,\\ & 0 \leq \tilde{y} \perp q + Nx + M\tilde{y} \geq 0,\end{aligned}$$

which is in the form of (2). To check if we can apply the techniques presented in Section 4, we have to analyze the definiteness of the matrix M. Since

$$\begin{pmatrix} y\\ z\\ \lambda\end{pmatrix}^\top \begin{bmatrix} 0 & 0 & 0\\ 0 & 0 & -C_3^\top\\ B_3 & C_3 & 0\end{bmatrix} \begin{pmatrix} y\\ z\\ \lambda\end{pmatrix} = \lambda^\top B_3 y$$

holds, the matrix M is, in general, indefinite. This means, that general linear trilevel problems cannot be tackled using the reformulations of the last section unless we make some additional assumptions.

Remark 8. (i) *If we consider the special case that the third level does not depend on the variables of the first level, we obtain $A_3 = 0$, which leads to $N = 0$. That is, we are in the case studied in Section 3. However, the indefiniteness of the matrix M is not affected by this simplification.*

(ii) *The situation changes if the third-level problem does not depend on the second-level variables. In this case, we have $B_3 = 0$ and the LCP matrix reduces to*

$$M = \begin{bmatrix} 0 & -C_3^\top\\ C_3 & 0\end{bmatrix},$$

which is a bisymmetric matrix. Since the $(1,1)$ block of M is zero and thus positive semidefinite, M is positive semidefinite as well and we can apply the techniques presented at the end of Section 4. This still holds if we generalize the linear objective function $e_3^\top z$ of the third level to a quadratic objective function of the form $e_3^\top z + 1/2 z^\top Qz$ with a positive semidefinite matrix Q. The bisymmetric LCP matrix then is given by

$$M = \begin{bmatrix} Q & -C_3^\top\\ C_3 & 0\end{bmatrix},$$

which is still positive semidefinite because Q is positive semidefinite. Finally, in this case, the trilevel model is not harder than an LPCC; see Remark 7.

6. Examples of Bilevel Problems with LPCC Lower-Levels in Transportation and Energy

In this section, we describe two important instances of the bilevel problem with an LPCC lower level. We focus on the following two problems: (i) a bilevel spatial price equilibrium model representing transportation of a product or service over a network with vehicles and (ii) a bilevel oligopoly model of the energy sector in its uncapacitated version.

These two general problems have the following structure that is also indicative of other examples such as sensor networks, traffic equilibrium, etc.

Top-level player: A federal (or regional) regulator, policy-maker, or another decision-maker at the system level.

Bottom-level players: A regional network operator who optimizes the lower-level objective function that is constrained by separate network users or market participants, whose interplay is modeled via complementarity constraints.

The spatial price equilibrium problem relates to an LCP that has no related optimization problem in its most general form due to the principle of symmetry (Gabriel et al. 2012). By contrast, the Nash–Cournot power market oligopoly is derived directly from considering a set of optimization problems. This distinction is important since it shows the breadth of the problems that we can solve. We anticipate that the resulting three-level infrastructure models—regulator (top level), network operator (middle level), and network users (lowest level)—will have broad applications in many infrastructure areas as indicated. However, also other engineering and economic applications are possible given the computationally tractable modeling approach we have outlined.

Within each of the following subsections, we also describe the conditions on the lower-level LCP matrix M that make it either positive definite or positive semidefinite.

6.1. **Bilevel Spatial Price Equilibrium.** We consider an instance of the spatial price equilibrium (SPE) problem (see, e.g., Gabriel et al. (2012)) on a complete bipartite graph with m supply points $S = \{1, \dots, m\}$ and n demand regions $D = \{1, \dots, n\}$. An equilibrium is a flow $y = (y_{ij})_{i \in S, j \in D}$ that solves the complementarity problem

$$0 \leq F_{ij}(y) \perp y_{ij} \geq 0 \quad \text{for all } i \in S,\ j \in D,$$

where

$$F_{ij}(y) = \psi_i \left(\sum_{j' \in D} y_{ij'} \right) + c_{ij}(y) - \theta_j \left(\sum_{i' \in S} y_{i'j} \right).$$

Here, $\psi_i(\sum_{j' \in D} y_{ij'})$ is the inverse supply function for supply node $i \in S$, $c_{ij}(y)$ are the transportation charges for sending flow from node $i \in S$ to node $j \in D$, and $\theta_j(\sum_{i' \in S} y_{i'j})$ is the inverse demand function for demand node $j \in D$. Thus, $\psi_i \left(\sum_{j' \in D} y_{ij'}\right) + c_{ij}(y)$ represents the delivered price in shipping the flow from node i to node j and $\theta_j \left(\sum_{i' \in S} y_{i'j}\right)$ is the marginal value of this flow at the destination market. If there is positive flow, i.e., if $y_{ij} > 0$, by complementarity, this means that this delivered price must be equal to the marginal value for that (i, j) pair. In what follows, we assume that the vector-valued function $F = (F_{ij})_{i \in S, j \in D}$ is affine in the flows y. This is accomplished by the following assumptions. First, the supply and demand functions are affine, i.e.,

$$\psi_i \left(\sum_{j' \in D} y_{ij'} \right) = a_i + b_i \left(\sum_{j' \in D} y_{ij'} \right) \quad \text{with} \quad a_i, b_i > 0 \quad \text{for all } i \in S$$

and

$$\theta_j \left(\sum_{i' \in S} y_{i'j} \right) = \alpha_j - \beta_j \left(\sum_{i' \in S} y_{i'j} \right) \quad \text{with} \quad \alpha_j, \beta_j > 0 \quad \text{for all } j \in D$$

holds. Second, the transportation charges have the form

$$c_{ij}(y) = c_{ij} = \eta_{ij} + \tau_{ij} \quad \text{for all } i \in S,\ j \in D,$$

where η_{ij} is an average vehicle operating cost for the route (i, j) and τ_{ij} is an emissions tariff imposed by the top-level regulator; see below for the details. The τ_{ij} tariffs are the main connection between the upper-level problem and the lower-level's LCP. However, there are other indirect connections as described below as well. Under the above assumptions, the resulting SPE is an LCP, whose (symmetric) matrix is positive semidefinite as shown in Theorem 10 below.

6.1.1. *Positive Semidefiniteness of the LCP Matrix M.* In the general setting of m supply and n demand nodes, the ith diagonal block matrix $M_{ii} \in \mathbb{R}^{n\times n}$, $i \in S$, is of the form

$$M_{ii} = \begin{bmatrix} b_i + \beta_1 & b_i & \cdots & b_i \\ b_i & b_i + \beta_2 & & b_i \\ \vdots & \vdots & \ddots & \vdots \\ b_i & b_i & \cdots & b_i + \beta_n \end{bmatrix}. \tag{8}$$

Moreover, all off-diagonal matrices are of the form $\Delta = \operatorname{diag}(\beta_1, \ldots, \beta_n) \in \mathbb{R}^{n\times n}$. Thus, the general form of the LCP matrix M is as follows:

$$M = \begin{bmatrix} M_{11} & \Delta & \Delta & \cdots & \Delta \\ \Delta & M_{22} & \Delta & \cdots & \Delta \\ \vdots & & \ddots & & \vdots \\ \Delta & \Delta & \Delta & \cdots & M_{mm} \end{bmatrix}. \tag{9}$$

Note that in each block row and block column of M, there are $m-1$ copies of the diagonal matrix Δ in the off-diagonal blocks. An important result relating to the positive semidefiniteness of M in (9) concerns the block matrix $\tilde{\Delta} \in \mathbb{R}^{mn\times mn}$ with all m^2 blocks are Δ.

Lemma 9. *The square matrix $\tilde{\Delta} \in \mathbb{R}^{mn\times mn}$ is positive definite for $m = 1$ and positive semidefinite for $m \geq 2$.*

Proof. For $m = 1$, $\tilde{\Delta}$ is a diagonal matrix with positive entries $\beta_1, \ldots, \beta_n$ so the result immediately follows. For $m \geq 2$, we consider the eigenvalue-eigenvector equation $\tilde{\Delta} y = \lambda y$, where $y = (y_1^\top, \ldots, y_m^\top)^\top$ is a non-zero vector with sub-vectors $y_i \in \mathbb{R}^n$ for all $i \in S$. We see that the ith block of equations reads

$$\Delta \left(\sum_{i \in S} y_i \right) = \lambda y_i.$$

The left-hand side is the same for all blocks $i = 1, \ldots, m$, which implies that $\lambda y_i = \lambda y_k$ for all $i, k \in S$. This in turn implies that $\lambda(y_i - y_k) = 0$ must hold which means that either $y_i = y_k$ or $\lambda = 0$. In the first case, this means that $m\Delta y_i = \lambda y_i$ holds, where $y_i \neq 0$, is the common sub-vector, i.e., $y_1 = \cdots = y_m$. It is easy to see that the eigenvalues λ are then just m times the diagonal entries of Δ, i.e., $m\beta_1, \ldots, m\beta_m$, which are all positive. Lastly, in the second case, $\lambda = 0$ which shows the desired result. □

The following result indicates that the LCP matrix in (9) is positive semidefinite.

Theorem 10. *Consider the symmetric matrix M given in (9). If $b_i > 0$, $\beta_j > 0$ hold for all $i \in S$, $j \in D$, then M is positive semidefinite.*

Proof. First note that the matrix M_{ii} in (8) can be split up as $M_{ii} = \Delta + b_i J$, where $J \in \mathbb{R}^{n\times n}$ is the matrix of all ones. Then, M in (9) can be re-arranged as follows:

$$M = \begin{bmatrix} \Delta & \cdots & \Delta \\ \vdots & \ddots & \vdots \\ \Delta & \cdots & \Delta \end{bmatrix} + \begin{bmatrix} b_1 J & 0 & 0 & \ldots & 0 \\ 0 & b_2 J & 0 & \ldots & 0 \\ \vdots & & \ddots & \ldots & \vdots \\ 0 & 0 & 0 & \ldots & b_m J \end{bmatrix}.$$

However, the first matrix is positive semidefinite as shown in Lemma 9 for $m \geq 2$ or positive definite for $m = 1$. Moreover, the second matrix is positive semidefinite since each matrix J has eigenvalues $\{0, \ldots, 0, n\}$, $b_i > 0$ for all $i \in S$, and given the block structure. The result then follows. □

6.1.2. *The Overall Bilevel Spatial Price Equilibrium Problem.* The lower-level LCP described above encompasses a distribution network in which some good or service is shipped from the supply to the demand nodes. A network operator is assumed to manage such a network but does not have direct control of the distribution pattern, allowing all supply and demand points to behave according to the lower-level SPE problem. Rather, this network operator is trying to minimize the total repair or maintenance costs of running this network with the costs given by σ_{ij} (exogenous data) for flow along route (i, j). Thus, the objective for the network operator is to minimize $\sum_{i\in S}\sum_{j\in D}\sigma_{ij}y_{ij}$.

Positioned above this network operator is a federal or regional regulator. This regulator decides policy on the transportation aspects of this distribution and other transport networks trying to trade off the costs of vehicle emissions with potential revenues from drivers choosing to go from origin i to destination j. Such a regulator decides on such things as vehicle-emissions costs to promote cleaner-burning vehicles. Thus, the regulator decides on a tariff τ_{ij} relating to emissions prices for the origin-destination pair (i, j) assuming fixed and exogenous emissions rates ε_{ij} for the OD (origin-destination) pair (i, j) and with κ the per-unit costs of cleaning up total emissions $(\sum_{i\in S}\sum_{j\in D}\varepsilon_{ij}y_{ij})$. The value $\tau_{ij} > 0$ can be considered as the average estimate of the clean-up costs of vehicles' emissions for the OD pair (i, j). The regulator also considers that on average, ω_{ij} dollars per volume of traffic will be generated from all the cities and towns visited in going from i to j. Here, we assume that $\omega_{ij} \geq \kappa\varepsilon_{ij}$ for at least one (i, j) to make positive flow reasonable from the perspective of the top-level player. For those OD pairs for which this is not the case, the top-level player can appropriately penalize with the emissions tariff τ_{ij}; see also the remark at the end of this section. In addition, the regulator wants to minimize the cost of emissions, given as the exogenous data κ dollars per ton with total emissions given as $\sum_{i\in S}\sum_{j\in D}\varepsilon_{ij}y_{ij}$.

Thus, the overall bilevel problem, with upper-level variables $\tau = (\tau_{ij})_{(i,j)\in S\times D}$, can be stated as

$$\max_{\tau} \quad \sum_{i\in S}\sum_{j\in D}\omega_{ij}y_{ij} - \kappa\left(\sum_{i\in S}\sum_{j\in D}\varepsilon_{ij}y_{ij}\right)$$
$$\text{s.t.} \quad \tau_{ij} \geq 0 \quad \text{for all } i \in S,\ j \in D,$$

where $y = (y_i)_{i\in S}$ with $y_i = (y_{ij})_{j\in D}$ solves the lower-level LPCC

$$\min_{y} \quad \sum_{i\in S}\sum_{j\in D}\sigma_{ij}y_{ij} \quad \text{s.t.} \quad 0 \leq My + q \perp y \geq 0.$$

Comparing this bilevel problem with the general form given in (1) and (2), we see that M is specified as in (9), with q further split up as

$$q = \begin{pmatrix} a_1 - \alpha_1 + \eta_{11} \\ a_1 - \alpha_2 + \eta_{12} \\ \vdots \\ a_m - \alpha_n + \eta_{mn} \end{pmatrix} + N\tau$$

with $N \in \mathbb{R}^{mn\times mn}$ being the identity matrix.

Remark 11. (i) *From the perspective of the top-level player, there is an incentive to have as much flow on each route (i, j) as possible to promote economic gain $\sum_{i\in S}\sum_{j\in D}\omega_{ij}y_{ij}$.*

(ii) *There is also a need to restrict flow on routes with high emissions ε_{ij}. The top-level player can increase emissions tariffs τ_{ij} to this end. Consider, for example, the OD pair (i, j). Note that*

$$F_{ij}(y) = a_i + b_i\left(\sum_{j\in D}y_{ij}\right) + \eta_{ij} + \tau_{ij} - \alpha_j + \beta_j\left(\sum_{i\in S}y_{ij}\right)$$

holds. If τ_{ij} is made sufficiently large by the top-level player, i.e., $\tau_{ij} > -a_i + \alpha_j - \eta_{ij}$ in combination with $b_i, \beta_j, y_{ij} \geq 0$, the resulting flow y_{ij} will equal 0 as determined by the complementarity conditions of the lower-level problem.

6.2. **A Bilevel Oligopoly Model of the Energy Sector.** We next consider a bilevel optimization problem with an energy oligopoly at the lower level for a set of energy firms $F = \{1, \dots, N_F\}$. At this lower level, these N_F firms constitute the entire electric power market for a given region. The oligopoly will be expressed as an LCP.

We consider the case of uncapacitated production. In our setting, every firm $i \in N_F$ decides on its own production level y_i and takes into account a linear inverse demand function $p(y_1, \dots, y_{N_F}) = \alpha - \beta(\sum_{i=1}^{N_F} y_i)$ with price intercept $\alpha > 0$ and slope $\beta > 0$; see for example, Gabriel et al. (2012).[3] Thus, the market price depends on the sum of the production of all firms. Each producing firm solves the profit-maximization problem

$$\max_{y_i} \quad p(y_1, \dots, y_{N_F}) y_i - \gamma_i y_i \quad \text{s.t.} \quad y_i \geq 0, \tag{10}$$

where γ_i is the marginal production cost for firm i that is composed of a firm-specific cost ζ_i and an emissions price π_i determined by the regulator, i.e., the top-level player. This emissions price is assumed to be exogenous to each of the firms and can vary by type of production; e.g., combined cycle gas turbine, coal power plant, etc. It is easy to see that the objective function of (10) is concave.[4] Thus, the KKT conditions are both necessary and sufficient. Taking the KKT conditions for all N_F firms together results in the LCP(q, M) in the variables $y_1, \dots, y_{N_F}$ that is given by

$$0 \leq \begin{bmatrix} 2\beta & \beta & \cdots & \beta \\ \beta & 2\beta & \cdots & \beta \\ \vdots & \vdots & \ddots & \vdots \\ \beta & \dots & \beta & 2\beta \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_F} \end{pmatrix} + \begin{pmatrix} \gamma_1 - \alpha \\ \gamma_2 - \alpha \\ \vdots \\ \gamma_{N_F} - \alpha \end{pmatrix} \perp \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_F} \end{pmatrix} \geq 0.$$

Here, the LCP vector is given by $q = (\gamma_1 - \alpha, \dots, \gamma_{N_F} - \alpha)^\top$ and the LCP matrix is

$$M = \begin{bmatrix} 2\beta & \beta & \cdots & \beta \\ \beta & 2\beta & \cdots & \beta \\ \vdots & \vdots & \ddots & \vdots \\ \beta & \dots & \beta & 2\beta \end{bmatrix}. \tag{11}$$

Theorem 12. *The symmetric matrix M in (11) is positive definite.*

Proof. Consider that M can be written as

$$M = \beta \begin{bmatrix} 2 & 1 & \cdots & 1 \\ 1 & 2 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 2 \end{bmatrix} = \beta(J + I).$$

Here, since J is a matrix of all ones, it has eigenvalues $\{0, \dots, 0, N_F\}$ and thus is positive semidefinite and I is the identity matrix, which is positive definite. Since β is positive, this shows the claim. □

The overall lower-level problem can be stated as follows assuming that the independent system operator (ISO) for the energy market in consideration wants to minimize total operational costs of the network stemming from power production. These costs of energy for

[3] It is implicitly assumed that costs and other factors may differ by index i representing different fuel-firm combinations. For example, an energy company that uses both coal and natural gas for power production would then be split into two separate firms using this notation.

[4] With $f_i(y_i) = -(p(y_1, \dots, y_{N_F}) y_i - \gamma_i y_i)$, the Hessian matrix $\nabla^2 f_i(y_i) = 2\beta > 0$ so that $f_i(y_i)$ is strictly convex.

the network operators are given as $\mu_i > 0$ and, for simplicity, we ignore any distributional constraints, e.g., related to power flow. Note that it is assumed that each firm i can refer to different types of production by an energy producer, e.g., combined cycle gas turbine vs. coal—hence the need for different emissions rates. Such a minimization should at least meet some minimum renewable production percentage $\rho \in [0,1]$ of the total electricity production. Thus, the lower-level LPCC is as follows, where $R \subseteq F$ with $|R| = N_R$ is the subset of firms that produce renewable energy (or divisions of firms if both renewable and non-renewable power for example is produced by the same firm):

$$\min_{y} \quad \mu^\top y \tag{12a}$$

$$\text{s.t.} \quad \sum_{i \in R} y_i \geq \rho \sum_{i \in F} y_i \tag{12b}$$

$$0 \leq \begin{bmatrix} 2\beta & \beta & \cdots & \beta \\ \beta & 2\beta & \cdots & \beta \\ \vdots & \vdots & \ddots & \vdots \\ \beta & \dots & \beta & 2\beta \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_F} \end{pmatrix} + \begin{pmatrix} \gamma_1 - \alpha \\ \gamma_2 - \alpha \\ \vdots \\ \gamma_{N_F} - \alpha \end{pmatrix} \perp \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_F} \end{pmatrix} \geq 0. \tag{12c}$$

On top of this lower level is the federal or regional regulator who tries to both promote renewable energy and the value of the total production. For each production level y_i, the top-level player assumes it will have a value of λ_i so that $\sum_{i \in F} \lambda_i y_i$ is to be maximized. On the other hand, for each non-renewable energy production level y_i, $i \in F \setminus R$, there is an associated emissions level η_i, i.e., $\sum_{i \in F \setminus R} \eta_i y_i$ is to be minimized.[5] The top-level player decides on emissions prices π_i, (again, i can refer to a type of energy by each firm) which figures into the variable costs for each firm. As noted above, $\gamma_i = \zeta_i + \pi_i$, where $\zeta_i > 0$ is the cost specific to the fuel-firm combination and π_i is the emissions price (fixed for the lower level) decided by the top-level player.

Given the upper-level variables $\pi = (\pi_i)_{i \in F} \in \mathbb{R}^{N_F}$, the overall bilevel problem is given by

$$\max_{\pi, y} \quad \sum_{i \in F} \lambda_i y_i - \sum_{i \in F \setminus R} \eta_i y_i \quad \text{s.t.} \quad \pi_i \geq 0 \quad \text{for all } i \in F,$$

where y solves (12).

Comparing this bilevel problem with the general form given in (1) and (2), we see that M is specified as in (11) and q is further split up as

$$q = \begin{pmatrix} \zeta_1 - \alpha_1 \\ \vdots \\ \zeta_{N_F} - \alpha_{N_F} \end{pmatrix} + Nx$$

with $N \in \mathbb{R}^{N_F \times N_F}$ being the identity matrix.

Remark 13. (i) *If π_i is chosen large enough, keeping in mind that $\beta \geq 0$ and $y_i \geq 0$ for all $i \in F$, then the complementarity function*

$$\beta y_i + \sum_{i \in F} \beta y_i + \zeta_i + \pi_i - \alpha_i > 0$$

for $i \in F$. Specifically, this is accomplished if $\pi_i > -\zeta_i + \alpha_i$. By the complementarity condition of the lower-level problem, this means that $y_i = 0$ holds so that the upper-level player can use the π_i values as a penalty for non-renewable production.

(ii) *On the other hand, forcing non-renewable power production to zero while maintaining feasibility for the minimum renewable power production percentage constraint*

[5] Without loss of generality, it is assumed that renewable production y_i, $i \in R$, has zero emissions, i.e., $\eta_i = 0$ for all $i \in R$.

may not be best from the perspective of maximizing the total value $\sum_{i \in F} \lambda_i y_i$*. Thus, there may be some incentive to produce some non-renewable energy.*

The model can be easily adapted to the capacitated case, in which the LCP matrix becomes positive semidefinite instead of positive definite.

7. Conclusion

In this paper, we introduced a novel class of bilevel optimization problems that have a lower level that is an LPCC. We derived single-level reformulations of these bilevel models that again contain complementarity constraints. Thus, these single-level reformulations can be useful in practice since they can be tackled using techniques similar to those used for single-level reformulations of, e.g., classic LP-LP bilevel problems. This is also the reason why we refrained from including a numerical case study since it, in the end, would rely on computational techniques that have been used and discussed in the literature of bilevel optimization many times.

We did not discuss the case of a lower-level LPCC with an indefinite LCP matrix. This case includes bilevel problems with (mixed-)integer lower-level models for which many novel solution techniques have been developed during the last years. However, studying these mixed-integer bilevel problems from the perspective of lower levels with indefinite LPCCs might lead to interesting novel approaches to tackle this even more challenging class of problems. This is part of our future research.

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