

A SURVEY ON MIXED-INTEGER PROGRAMMING TECHNIQUES IN BILEVEL OPTIMIZATION

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ABSTRACT. Bilevel optimization is a field of mathematical programming in which some variables are constrained to be the solution of another optimization problem. As a consequence, bilevel optimization is able to model hierarchical decision processes. This is appealing for modeling real-world problems, but it also makes the resulting optimization models hard to solve in theory and practice. The scientific interest in computational bilevel optimization increased a lot over the last decade and is still growing. Independent of whether the bilevel problem itself contains integer variables or not, many state-of-the-art solution approaches for bilevel optimization make use of techniques that originate from mixed-integer programming. These techniques include branch-and-bound methods, cutting planes and, thus, branch-and-cut approaches, or problem-specific decomposition methods. In this survey article, we review bilevel-tailored approaches that exploit these mixed-integer programming techniques to solve bilevel optimization problems. To this end, we first consider bilevel problems with convex or, in particular, linear lower-level problems. The discussed solution methods in this field stem from original works from the 1980's but, on the other hand, are still actively researched today. Second, we review modern algorithmic approaches to solve mixed-integer bilevel problems that contain integrality constraints in the lower level. Moreover, we also briefly discuss the area of mixed-integer nonlinear bilevel problems. Third, we devote some attention to more specific fields such as pricing or interdiction models that genuinely contain bilinear and thus nonconvex aspects. Finally, we sketch a list of open questions from the areas of algorithmic and computational bilevel optimization, which may lead to interesting future research that will further propel this fascinating and active field of research.

1. INTRODUCTION

In this paper, we consider bilevel optimization problems of the general form

$$\min_{x \in X, y} F(x, y) \tag{1a}$$

$$\text{s.t. } G(x, y) \geq 0, \tag{1b}$$

$$y \in S(x), \tag{1c}$$

where $S(x)$ is the set of optimal solutions of the x -parameterized problem

$$\min_{y \in Y} f(x, y) \tag{2a}$$

$$\text{s.t. } g(x, y) \geq 0. \tag{2b}$$

Problem (1) is the so-called upper-level (or the leader's) problem and Problem (2) is the so-called lower-level (or the follower's) problem. Moreover, the variables $x \in \mathbb{R}^{n_x}$ are the upper-level variables (or leader's decisions) and $y \in \mathbb{R}^{n_y}$ are lower-level

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variables (or follower’s decisions). The objective functions are given by $F, f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \rightarrow \mathbb{R}$ and the constraint functions by $G : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \rightarrow \mathbb{R}^m$ as well as $g : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \rightarrow \mathbb{R}^\ell$. The sets $X \subseteq \mathbb{R}^{n_x}$ and $Y \subseteq \mathbb{R}^{n_y}$ are typically used to denote integrality constraints. For instance, $Y = \mathbb{Z}^{n_y}$ makes the lower-level problem an integer program. In what follows, we call upper-level constraints $G_i(x, y) \geq 0$, $i \in \{1, \dots, m\}$, coupling constraints if they explicitly depend on the lower-level variable vector y . Moreover, all upper-level variables that appear in the lower-level constraints are called linking variables.

We use the nomenclature that the bilevel problem (1) is called an “UL-LL problem” where UL and LL can be LP, QP, MILP, MIQP, etc. if the upper-/lower-level problem is a linear, a quadratic, a mixed-integer linear, a mixed-integer quadratic, etc. program in both the variables of the leader and the follower. If the concrete specification of both levels is not required, we also use a shorter nomenclature and say, e.g., that the problem is a bilevel LP, if both levels are LPs.

Most of the time, we will consider the optimistic version of the bilevel problem as it is given in (1). In this case, the leader also optimizes over the lower-level outcome $y \in S(x)$ if the lower-level solution set $S(x)$ is not a singleton. On the contrary, the pessimistic version is given by

$$\min_{x \in X} \max_{y \in S(x)} F(x, y) \quad \text{s.t.} \quad G(x, y) \geq 0 \text{ for all } y \in S(x).$$

For the general pessimistic setting, we refer to Wiesemann et al. (2013) and the recent surveys on pessimistic bilevel optimization in Liu, Fan, et al. (2018) and Liu, Fan, et al. (2020).

Instead of using the point-to-set mapping S one can also use the so-called optimal value function

$$\varphi(x) := \min_{y \in Y} \{f(x, y) : g(x, y) \geq 0\} \tag{3}$$

and re-write Problem (1) as

$$\min_{x \in X, y \in Y} F(x, y) \tag{4a}$$

$$\text{s.t.} \quad G(x, y) \geq 0, \quad g(x, y) \geq 0, \tag{4b}$$

$$f(x, y) \leq \varphi(x), \tag{4c}$$

to which we will refer as the value-function reformulation. This reformulation indicates that for the optimistic version of the problem, we can assume without loss of generality that all upper-level variables are linking variables; see Bolusani and Ralphs (2020).

Bilevel optimization problems date back to the seminal publications on leader-follower games of von Stackelberg (1934, 1952). The introduced formulation was first used in Bracken and McGill (1973) in the context of a military application regarding the cost-minimal mix of weapons. Another very early discussion of multilevel, or, in particular, two-level problems can be found in Candler and Norton (1977). Over the years, bilevel optimization has been recognized as an important modeling tool since it allows to formalize hierarchical decision processes that often appear in application areas such as energy, security, or revenue management. We postpone the discussion of selected applied literature to the following sections.

The ability to model hierarchical decision processes also makes bilevel optimization problems notoriously hard to solve. For instance, already their easiest instantiation with a linear upper- and lower-level problem is strongly NP-hard; see Section 3 for the details. Thus, efficient, i.e., polynomial-time, algorithms cannot be expected unless $P = NP$. This also makes the development of solution algorithms a difficult task on the one hand—but on the other hand “allows” for enumeration-based algorithms such as branch-and-bound. During the last years and decades it turned out that

the development of solution algorithms for bilevel optimization problems strongly depends on the structure and properties of the lower-level problem as well as on the coupling between the upper and the lower level. For instance, the solution techniques are very much different depending on whether the lower-level problem is continuous and convex or whether it is nonconvex, e.g., due to the presence of integer variables.

In this survey, we focus on algorithmic techniques to actually solve bilevel problems. In particular, we discuss techniques from mixed-integer linear or nonlinear optimization that are applied in the field of bilevel optimization. These basic and well-studied techniques include branch-and-bound (Land and Doig 1960) or cutting planes (Kelley 1960) as well as decomposition techniques such as (generalized) Benders decomposition (Benders 1962; Geoffrion 1972); see the books by Conforti et al. (2014), Jünger et al. (2010), and Wolsey (1998) for a comprehensive overview about mixed-integer linear programming techniques. Moreover, also specific techniques from mixed-integer nonlinear programming such as outer approximation (Bonami et al. 2008; Duran and Grossmann 1986; Fletcher and Leyffer 1994) or spatial branching (Horst and Tuy 2013) are covered; see Belotti et al. (2013) and Lee and Leyffer (2012) for recent overviews on mixed-integer nonlinear optimization. For the more theoretical aspects of bilevel optimization we refer to Dempe (2002) and the references therein.

Obviously, the entire field of bilevel optimization is much broader and we thus are not able to cover everything. For instance, we do not cover the fields of bilevel optimization under uncertainty (Besançon et al. 2019, 2020; Burtscheidt and Claus 2020; Burtscheidt, Claus, and Dempe 2020; Dempe, Ivanov, et al. 2017; Ivanov 2018; Jain, Ordóñez, et al. 2008; Pita, Jain, Tambe, et al. 2010; Yanikoglu and Kuhn 2018), fractional bilevel optimization (Calvete and Galé 1999, 2004), or purely continuous nonconvex bilevel problems (Dempe, Mordukhovich, et al. 2019; Fliege et al. 2020).

Finally, let us mention already existing surveys (Colson et al. 2007; Colson et al. 2005) and books (Bard 1998; Dempe 2002; Dempe, Kalashnikov, et al. 2015) in the field of bilevel optimization. Other very early survey articles include Anandalingam and Friesz (1992), Ben-Ayed (1993), Kolstad (1985), and Vicente and Calamai (1994) as well as Wen and Hsu (1991) regarding the field of linear bilevel optimization. Last but not least, Dempe (2020) contains, to the best of our knowledge, the largest annotated list of references in the field of bilevel optimization.

The remainder of this survey is structured as follows. In Section 2, we collect selected applications from various different fields to motivate the study of bilevel problems. Afterward, in Section 3, we discuss bilevel optimization problems with linear or, at least, convex lower-level problems. For this problem class, we study important general properties, derive classical single-level reformulations, and give a comprehensive overview of the algorithms used to solve these problems. The case of bilinear bilevel problems is discussed in Section 4, where we focus on pricing problems and Stackelberg games. In Section 5, we then turn to bilevel problems with mixed-integer (non)linear lower-level problems. Also for these problems, we first focus on general properties before we then turn to generic approaches for solving bilevel MILPs and bilevel MINLPs. Section 6 is then devoted to interdiction problems. Here, we discuss both discrete as well as continuous interdiction problems, different fields of applications, and different classes of algorithms to tackle these problems. The survey closes with a collection of possible directions for future research in Section 7.

2. SELECTED APPLICATIONS

In this section, we present a selection of the vast literature on applications of bilevel optimization. Due to the enormous number of publications, this review will be far from being comprehensive. Many other application-oriented papers can, e.g., be found in the survey by Dempe (2020) or by Sinha, Malo, and Deb (2018).

Early Applications. Among the first, bilevel optimization has been applied to military defense problems in Bracken and McGill (1973) and to agricultural planning; see Candler, Fortuny-Amat, et al. (1981) and Fortuny-Amat and McCarl (1981). The latter topic is also picked up in Bard, Plummer, et al. (2000). Recent references concerning the defense of critical infrastructure (Alguacil et al. 2014; Borrero et al. 2019; Caprara et al. 2016; DeNegre 2011; Fioretto et al. 2019; Scaparra and Church 2008; Wood 2011) are related to the mentioned early military applications. Many of these bilevel problems were originally considered in the field of game theory and are thus often called Stackelberg games. A particular attention has been given to those involving a finite number of strategies; see, e.g., Sections 4.2 and 6.

Other early applications can be found in chemical process design that involves thermodynamic equilibria; see, e.g., Clark and Westerberg (1983), Clark and Westerberg (1990), Clark (1990), and Gümüş and Ciric (1997).

Traffic and Transportation. Bilevel traffic and transportation planning problems are covered, among others, in LeBlanc and Boyce (1986), Marcotte (1986), Ben-Ayed, Boyce, et al. (1988), Ben-Ayed, Blair, et al. (1992), and Migdalas (1995), as well as more recently in Fontaine and Minner (2014) or Gairing et al. (2017). Usually, the upper level models the decisions on the transportation network design, while the lower level models the individual behavior of the users of the network. Additionally, bilevel optimization is also used for the detection and solution of aircraft conflicts (Cerulli, D’Ambrosio, et al. 2019; Cerulli, d’Ambrosio, et al. 2020), for which tailored cutting planes are proposed.

Management Science. In the context of management science, in Bard (1983), bilevel optimization is used to coordinate multi-divisional firms. Further, Ryu et al. (2004) address bilevel decision-making problems under uncertainty in the context of enterprise-wide supply chain optimization, Garcia-Herreros et al. (2016) consider bilevel capacity expansion planning problems, and Reisi et al. (2019) and Yue and You (2017) consider supply chain problems. In Dan, Lodi, et al. (2020) and Dan and Marcotte (2019), the authors consider service firms deciding on the location and service levels of its facilities, taking into account the behavior of the user. This results in mixed-integer nonlinear bilevel problems, for which tailored approaches are provided. Finally, bilevel portfolio optimization problems are considered in, e.g., González-Díaz et al. (2020) and Leal et al. (2020).

Machine Learning. Bilevel problems are also discussed in the context of statistics and machine learning. In Bennett, Jing Hu, et al. (2006) and Bennett, Kunapuli, et al. (2008), bilevel optimization is applied to hyper-parameter selection for statistical learning methods. An evolutionary bilevel algorithm for the same purpose is given in Sinha, Malo, Xu, et al. (2014). Very recently, Franceschi et al. (2018) introduce a framework based on bilevel programming that unifies gradient-based hyper-parameter optimization and meta-learning.

Energy Networks and Markets. Arguably, energy networks and markets are two of the largest areas of application; see, e.g., the book of Gabriel et al. (2012) with many applications and models. Some selected contributions that particularly consider electricity networks and markets are given in the following. Arroyo (2010)

analyze the vulnerability of power systems and Motto et al. (2005) analyze the security of power grids under disruptive threats. Problems of generation and transmission expansion planning are studied in Garcés et al. (2009), Jenabi et al. (2013), or Jin and Ryan (2011). See also Bylling et al. (2020) for a stochastic bilevel model in this context. In Grimm, Martin, et al. (2016), the authors propose a problem-tailored solution approach based on binary search to solve a similar problem. Further, Baringo and Conejo (2012) deal with transmission and wind power investment. Optimal placement of measurement devices in an electrical network has been modeled as a bilevel MILP in Poirion et al. (2020). The authors develop a generic branch-and-cut procedure that can be applied to problems with a similar type of bilevel constraints. Grimm, Kleinert, et al. (2019) and Kleinert and Schmidt (2019b) develop a Benders-like decomposition approach to compute optimal price zones of electricity markets. The approach is applied to the German electricity market in Ambrosius et al. (2020). Ruiz and Conejo (2009) consider a strategic power producer that trades electric energy in an electricity pool. Similarly, the equilibria reached by strategic producers in a pool-based network-constrained electricity market are studied in Ruiz, Conejo, and Smeers (2012) and Fampa et al. (2008) analyze strategic pricing in competitive electricity markets. Other works consider demand-side management (Aussel et al. 2020; Grimm, Orlinkskaya, et al. 2020), the scheduling of maintenance outages of a set of transmission lines (Pandzic et al. 2012), or how to economically exploit wind resources at a given location from a transmission-cost perspective (Morales et al. 2012). For a recent survey on bilevel optimization in energy and electricity markets see Wogrin et al. (2020). Besides electricity, gas markets are addressed by bilevel optimization as well; see, e.g., Böttger et al. (2020), Grimm, Schewe, et al. (2019), and Schewe et al. (2020) for models of the European entry-exit gas market.

3. CONTINUOUS LINEAR AND/OR CONVEX LOWER-LEVEL PROBLEMS

The general form of an LP-LP bilevel problem, i.e., a bilevel problem in which all constraints and objective functions are linear, is as follows:

$$\min_{x,y} c_x^\top x + c_y^\top y \quad (5a)$$

$$\text{s.t. } Ax + By \geq a, \quad (5b)$$

$$y \in \arg \min_{\bar{y}} \{d^\top \bar{y} : Cx + D\bar{y} \geq b\} \quad (5c)$$

with $c_x \in \mathbb{R}^{n_x}$, $c_y, d \in \mathbb{R}^{n_y}$, $A \in \mathbb{R}^{m \times n_x}$, $B \in \mathbb{R}^{m \times n_y}$, and $a \in \mathbb{R}^m$ as well as $C \in \mathbb{R}^{\ell \times n_x}$, $D \in \mathbb{R}^{\ell \times n_y}$, and $b \in \mathbb{R}^\ell$. Note that we already omitted a linear term depending on the upper-level variables x in the lower-level objective function since this term would not have any influence on the optimal solutions of the lower level. Moreover, for the ease of presentation, we always use linear lower-level problems if this is suitable to describe the general ideas and only use nonlinear but convex lower-level problems if this is required.

3.1. General Properties. We introduce two concepts that are useful to derive solution algorithms since they lead to bounds on the optimal value of bilevel problems. First, we consider the feasible region H of the so-called high-point relaxation (HPR), which is defined as the set of points (x, y) satisfying the leader and follower constraints, i.e., for Problem (5) it is given by

$$H := \{(x, y) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} : Ax + By \geq a, Cx + Dy \geq b\}.$$

Clearly, the solution of the HPR

$$\min_{x,y} \{c_x^\top x + c_y^\top y : (x, y) \in H\} \quad (6)$$

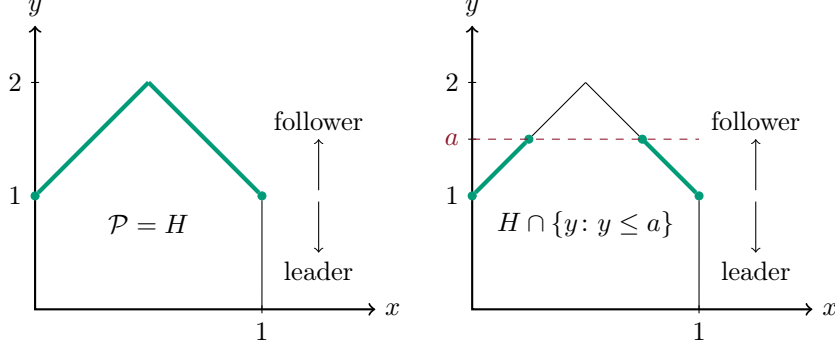


FIGURE 1. Illustration of the example in Section 3.1.

provides a lower bound on the optimal objective value of the bilevel problem, because it relaxes the optimality of the lower-level problem (5c). Second, we consider the bilevel feasible region \mathcal{F} , which is also denoted as the “inducible region” of the bilevel problem. This set particularly takes the optimal response of the follower into account and is given by

$$\mathcal{F} := \{(x, y) \in H : y \text{ satisfies (5c)}\}.$$

Having this notion at hand, we can write the bilevel LP (5) as

$$\min_{x,y} \{c_x^\top x + c_y^\top y : (x, y) \in \mathcal{F}\}.$$

This implies that any bilevel feasible point provides an upper bound on the optimal value of the bilevel LP.

To better understand the special features and properties of bilevel LPs, we illustrate them with some graphical examples involving one variable at each level. The problem

$$\min_{x,y} \left\{ y : y \in \arg \min_{\bar{y}} \{-\bar{y} : (x, \bar{y}) \in \mathcal{P}\} \right\},$$

with the lower level’s feasible region given by

$$\mathcal{P} = \{(x, y) : y \geq 0, y \leq 1 + x, y \leq 3 - x, 0 \leq x \leq 1\},$$

is depicted in Figure 1 (left). The feasible points of the HPR coincide with the lower-level feasible region \mathcal{P} since there are no upper-level constraint. The horizontal segment linking the origin and point $(1, 0)$ constitutes the set of solutions of the high-point relaxation, i.e., those points in H that minimize the upper-level objective function. Since the corresponding upper-level objective function is 0 on this segment, this leads to a lower bound of 0 for the entire bilevel LP. The bilevel feasible region \mathcal{F} is given by the union of the two segments in thick green. Interestingly, \mathcal{F} is nonconvex although both levels are linear optimization problems. The problem has the two optimal solutions $(0, 1)$ and $(1, 1)$ with value 1.

Now, if we add the constraint $y \leq a$ with $1 < a < 2$ to the upper level, the bilevel feasible region is reduced to two disjoint segments as depicted in Figure 1 (right). Nonetheless, these segments constitute faces of the high-point relaxation. An even worse situation may happen if the right-hand side of the constraint added to the upper level is set to $a \in (0, 1)$. Then, the bilevel feasible region is empty, i.e., the bilevel LP has no feasible point, although the high-point relaxation is feasible. This last example is also useful to illustrate the effect of moving coupling constraints, i.e., upper-level constraints involving variables of the lower level, between the two levels. If, e.g., the constraint $y \leq 1/2$ is added to the lower level, then the problem

becomes feasible and all points $(x, 1/2)$ with $0 \leq x \leq 1$ are bilevel optimal. The two facts that (i) coupling constraints of a bilevel LP may lead to a disconnected bilevel feasible region and that (ii) they cannot be moved to the lower level without changing the set of optimal solutions have been discussed by Audet, Haddad, et al. (2006) and Mersha and Dempe (2006).

Another interesting property is that the unboundedness of the HPR (6) does not allow to conclude about the optimal solution of the bilevel problem. An illustrative example, borrowed from Xu (2012) and Xu and Wang (2014) and slightly simplified here, demonstrates three different situations, in each of which the HPR solution is unbounded, but, depending on the objective function of the lower-level problem, the bilevel problem is either unbounded, infeasible, or admits an optimal solution. To this end, consider the bilevel problem

$$\begin{aligned} \max_{x,y} \quad & x + y \\ \text{s.t.} \quad & 0 \leq x \leq 2, \\ & y \in \arg \max_{y'} \{dy' : y' \geq x\} \end{aligned}$$

and its high-point relaxation

$$\begin{aligned} \max_{x,y} \quad & x + y \\ \text{s.t.} \quad & 0 \leq x \leq 2, \\ & y \geq x. \end{aligned}$$

For $d = 0$, the bilevel problem is unbounded as the lower-level problem is feasible for all y . For $d = 1$, the bilevel problem is infeasible, as $\varphi(x) = \infty$. Finally, for $d = -1$, the problem admits a unique optimal solution $(x, y) = (2, 2)$.

Despite the rather complicating properties of H and \mathcal{F} that we described above, the two sets can be exploited algorithmically. The groundwork for this is laid in Bialas and Karwan (1984) and Bard (1984). For the ease of exposition, let us assume that H is bounded and nonempty for what follows. In the following, we will explain that the bilevel feasible region is a union of faces of the high-point relaxation and that a bilevel optimal solution is attained at one of the vertices of this union. This is already illustrated in the previous example. A point (x, y) belonging to the bilevel feasible region \mathcal{F} must satisfy all constraints defining the polyhedron H and must be an optimal solution of the lower-level LP. Thus, (x, y) must satisfy the Karush–Kuhn–Tucker (KKT; see, e.g., Nocedal and Wright (2006)) conditions of the lower-level LP, which imply that each constraint is either active at (x, y) or that the corresponding dual variable is equal to 0. Consider now the face F of the polyhedron H obtained by setting all constraints active at point (x, y) at equality. All points on F also satisfy the KKT conditions for a dual solution corresponding to (x, y) implying that $F \subseteq \mathcal{F}$. This property implies that a bilevel LP possesses an optimal solution that is a vertex of H and that it can be found by solving an LP whose objective function is given by (5a) over each (maximal) face of H included in the bilevel feasible region.

The so-called K^{th} -Best algorithm proposed by Bialas and Karwan (1984) searches for a vertex of H that is optimal for the bilevel LP by starting with a vertex that minimizes (5a) and then iteratively generates adjacent vertices with nondecreasing value for (5a) until a vertex belonging to the bilevel feasible region is found. In the worst case, the K^{th} -Best algorithm requests to visit an exponential number of vertices of H (remember that the bilevel feasible region may be empty even though H is not). This is not surprising as Hansen et al. (1992) have shown that bilevel LPs are strongly NP-hard (see also Jeroslow (1985) for NP-hardness) by reducing the graph problem KERNEL and Vicente, Savard, et al. (1994) have shown that

even checking local optimality of a given point is NP-hard. In the same vein, Audet, Hansen, et al. (1997) remark that a binary constraint, say $x \in \{0, 1\}$, appearing in a single-level optimization problem can be modeled by an additional variable y and the constraints $y = 0$ and

$$y = \arg \max_{\bar{y}} \{\bar{y} : \bar{y} \leq x, \bar{y} \leq 1 - x\}.$$

As a consequence, linear optimization problems with binary variables are a special case of bilevel LPs. Further hardness results are also stated in Bard (1991), where some general properties of bilevel LPs are discussed as well. A survey about complexity results for bilevel LP problems can be found in Deng (1998). The strongest complexity result was obtained by Jeroslow (1985), who proved hardness of multilevel LP problems. Specifically, he showed that a k -level LP problem belongs to the complexity class Σ_{k-1}^P .

Finally, given that the objective functions of both levels play a role in a bilevel problem, it would be tempting to conclude that the optimal solution of a bilevel LP is Pareto-optimal with respect to these objectives. However, Marcotte and Savard (1991) have shown that this is not true unless c_y and d are parallel.

3.2. Single-Level Reformulations. If the lower-level problem of the bilevel optimization model at hand is convex and satisfies a suitable constraint qualification (which, in the convex case, usually is Slater's constraint qualification), then one can reformulate the bilevel problem into a single-level optimization problem. To this end, one either uses the KKT conditions of the lower-level problem or a strong duality theorem applied to the lower-level problem. In this section, we discuss both approaches and restrict ourselves, for the ease of presentation, to the case of LP-LP bilevel problems of the type given in (5). The lower-level problem (5c) can be seen as the x -parameterized linear problem

$$\min_y \quad d^\top y \quad \text{s.t.} \quad Dy \geq b - Cx. \quad (7)$$

Its Lagrangian function is given by

$$\mathcal{L}(y, \lambda) = d^\top y - \lambda^\top (Cx + Dy - b)$$

and the KKT conditions are given by dual feasibility

$$D^\top \lambda = d, \quad \lambda \geq 0,$$

primal feasibility

$$Cx + Dy \geq b,$$

and the KKT complementarity conditions

$$\lambda_i (C_i \cdot x + D_i \cdot y - b_i) = 0 \quad \text{for all } i = 1, \dots, \ell.$$

Here and in what follows, C_i denotes the i th row and $C_{\cdot j}$ denotes the j th column of C . Since the lower-level feasible region is polyhedral, the Abadie constraint qualification holds and the KKT conditions are both necessary and sufficient. Thus, the LP-LP bilevel problem can be reformulated as

$$\min_{x, y, \lambda} \quad c_x^\top x + c_y^\top y \quad (8a)$$

$$\text{s.t.} \quad Ax + By \geq a, \quad Cx + Dy \geq b, \quad (8b)$$

$$D^\top \lambda = d, \quad \lambda \geq 0, \quad (8c)$$

$$\lambda_i (C_i \cdot x + D_i \cdot y - b_i) = 0 \quad \text{for all } i = 1, \dots, \ell. \quad (8d)$$

Note that we now optimize over an extended space of variables since we additionally have to include the lower-level dual variables λ . Since we optimize over x , y , and λ simultaneously, any global solution of (8) is an optimistic bilevel solution. Problem (8)

is linear except for the KKT complementarity conditions that turn the problem into a nonconvex and nonlinear optimization problem (NLP). More precisely, Problem (8) is a mathematical program with complementarity constraints (MPCC); see, e.g., Luo et al. (1996). Unfortunately, standard NLP algorithms usually cannot be applied for such problems since classical constraint qualifications like the Mangasarian–Fromowitz or the linear independence constraint qualification are violated at every feasible point; see, e.g., Ye and Zhu (1995). For a primer on constraint qualifications in nonlinear optimization, see, e.g., the seminal textbook by Nocedal and Wright (2006). The inherent violation of suitable constraint qualifications for MPCCs lead to the development of both (i) tailored constraint qualifications and stationarity concepts (Hoheisel et al. 2013) as well as (ii) special solution techniques. However, the latter can achieve at most (if at all) local solutions of the MPCC. We refer the reader to Dempe (1987) and Still (2002), where this is used to solve the underlying bilevel problem to local optimality.

Besides this approach based on the lower level’s KKT conditions, one can also use a strong duality theorem for the lower-level problem. The dual problem to (7) is given by

$$\max_{\lambda} (b - Cx)^\top \lambda \quad \text{s.t.} \quad D^\top \lambda = d, \lambda \geq 0. \quad (9)$$

For a given decision x of the leader, weak duality of linear optimization states that

$$d^\top y \geq (b - Cx)^\top \lambda$$

holds for every primal and dual feasible pair y and λ . Thus, by strong duality, we know that every such feasible pair is a pair of optimal solutions if

$$d^\top y \leq (b - Cx)^\top \lambda$$

holds. Consequently, we can reformulate the bilevel problem as

$$\min_{x,y,\lambda} c_x^\top x + c_y^\top y \quad (10a)$$

$$\text{s.t.} \quad Ax + By \geq a, \quad Cx + Dy \geq b, \quad (10b)$$

$$D^\top \lambda = d, \quad \lambda \geq 0, \quad (10c)$$

$$d^\top y \leq (b - Cx)^\top \lambda. \quad (10d)$$

Here, the ℓ KKT complementarity constraints in (8) are replaced with the scalar inequality in (10d). Note that the general nonconvexity of LP-LP bilevel problems is reflected in this single-level reformulation due to the bilinear products of the primal upper-level variables x and the dual lower-level variables λ .

Let us close this section with a remark on single-level reformulations of problems more general than LP-LP bilevel problems. Both reformulations discussed can be applied as long as compact global optimality certificates for the lower level are available. This is, in general, the case if the lower-level problem is convex and if Slater’s constraint qualification holds. However, both the MPCC (8) and the nonconvex problem (10) are only equivalent to the original bilevel problem if globally optimal solutions are considered and if Slater’s constraint qualification holds. In particular, locally optimal solutions of Problem (8) are not necessarily locally optimal for the original bilevel problem; see Dempe and Dutta (2012) for the details.

3.3. Algorithms. The most likely earliest published paper on mixed-integer programming techniques for bilevel optimization is the one by Fortuny-Amat and McCarl (1981). The authors consider a bilevel optimization problem with a quadratic programming problem (QP) in the upper and the lower level. For the ease of presentation, we explain the core ideas based on the LP-LP bilevel problem (5). The authors first derive the single-level reformulation (8) based on the lower-level’s KKT

conditions and then linearize the KKT complementarity conditions (8d) by using additional binary variables. The key idea here is to consider the complementarity conditions $\lambda_i(C_i.x + D_i.y - b_i) = 0$, $i = 1, \dots, \ell$, as disjunctions stating that either $\lambda_i = 0$ or $C_i.x + D_i.y = b_i$ needs to hold. These two cases can be modeled using binary variables $z_i \in \{0, 1\}$, $i = 1, \dots, \ell$, in the following mixed-integer linear way,

$$\lambda_i \leq M_i^d z_i, \quad C_i.x + D_i.y - b_i \leq M_i^p (1 - z_i),$$

with sufficiently large constants M_i^d and M_i^p for the dual variable and the primal constraint. Consequently, $z_i = 1$ models the case that the primal inequality is active, whereas $z_i = 0$ models the inactive case in which the dual variable is zero. The resulting MILP reformulation can then be solved by general-purpose solvers. Unfortunately, this reformulation has a severe disadvantage because one needs to determine a big- M constant that both is valid for the primal constraint as well as for the dual variable. The primal validity is usually ensured by the assumption that the high-point relaxation is bounded, which is typically justified in practical applications. However, the dual feasible set is unbounded for bounded primal feasible sets; see Clark (1961) and Williams (1970). Thus, it is rather problematic to bound the dual variables of the follower. In practice, often “standard” values such as 10^6 are used without any theoretical justification or heuristics are applied to compute a big- M value, e.g., in Pineda, Bylling, et al. (2018), big- M values are determined from local solutions of the MPCC (8). In Pineda and Morales (2019) it is shown by an illustrative counter-example that such heuristics may deliver invalid values. Moreover, validating the correctness of a given big- M is shown to be NP-hard in general in Kleinert, Labbé, et al. (2020b).

All the mentioned methods so far solve a certain reformulation of the bilevel problem with general-purpose solvers. In addition, one can also develop bilevel-tailored solution techniques. Already in their paper from 1981, Fortuny-Amat and McCarl briefly discuss the possibility to set up a bilevel-specific branch-and-bound scheme. In this scheme, Problem (8) without the KKT complementarity conditions (8d) is solved at the root node. Afterward, it is checked whether all KKT complementarity conditions are satisfied. If not, the most violated one is chosen and two subproblems are constructed with either $\lambda_j = 0$ or $C_j.x + D_j.y = b_j$ added as a constraint if $j \in \{1, \dots, \ell\}$ is the most violated condition. In this manner, the method proceeds as a usual branch-and-bound method. This method is also used in Bard and Moore (1990), where it is computationally evaluated for bilevel problems with LP upper-level problems and lower-level problems that are convex QPs. Note that for convex QPs in the lower level, all problems to be solved in the nodes of the branch-and-bound tree are convex, which would not be the case anymore if bilinear terms as products of upper- and lower-level variables are present in the lower level. A very similar branch-and-bound algorithm for continuous bilevel problems is presented in Bard (1988). Here, bilevel problems with strictly convex upper-level objective function, convex quadratic lower-level objective function, polyhedral feasible set of the upper level, and convex feasible region of the lower level are considered. Moreover the lower-level problem needs to satisfy a suitable constraint qualification. Another extension of Bard and Moore (1990) for nonlinear but convex problems is given in Edmunds and Bard (1991). A branching rule different from most-violated complementarity is discussed in Hansen et al. (1992). At this point in time, problems with 250 leader variables, 150 follower variables, and 150 follower constraints were the largest instances that have been solved. Finally, we note that it is already stated in Fortuny-Amat and McCarl (1981) that the complementarity conditions can also be modeled as special ordered sets (SOS) of type 1; see Beale and Tomlin (1970). Modern mixed-integer solvers can handle SOS1 conditions out-of-the-box such that it is not necessary to implement the branching on complementarity conditions. The

branching rule is then left to the solver. This approach is also proposed by Siddiqui and Gabriel (2013) in an MPEC context and by Pineda, Bylling, et al. (2018) in a bilevel context.

In the history of integer programming, the basic branch-and-bound method has been extended to the so-called branch-and-cut (B&C) method. This means that, besides branching, additional valid inequalities or cuts are introduced at the nodes of the branch-and-bound tree to tighten the formulation. Whereas the literature on cutting planes in integer programming is huge, there are only a few papers dealing with valid inequalities in the bilevel case.

In Audet, Haddad, et al. (2007), the complementarity conditions (8d) have been used to obtain so called disjunctive cuts that are applied at the root node of the branch-and-bound tree. For each violated complementarity constraint, solving a linear optimization problem yields such a cut. In a small example, the usefulness of the cut is demonstrated. It is also shown that sometimes this cut couples primal feasibility (8b) and dual feasibility (8c) and sometimes it does not.

In Audet, Savard, et al. (2007), three further cuts are presented that can again be derived from the solution of the root node problem. The first one is a Gomory-like cut. For each violated complementarity constraint of the lower level, two inequalities can be derived. One of them is acting on the primal upper- and lower-level variables and the other one on the dual lower-level variables. The presentation of these inequalities is rather technical and we thus refer to the paper for the details. At least one of the two inequalities must be valid and is actually a cut. Since the valid one is not known, both inequalities are added to the problem and a binary switching variable is used to select the valid inequality. In this light, the two inequalities add a rather implicit coupling of the constraints (8b) and (8c). Another variant are so-called extended cuts that, similar to the Gomory-like cuts, also involve binary switching variables. However, it is noted that these cuts are deeper than the Gomory-like cuts. One can also derive two cuts that do not involve a switching variable. These cuts are called simple cuts in Audet, Savard, et al. (2007). Again, the combination of both cuts implicitly couples the primal upper and lower level with the dual lower level. In a small numerical study it is shown that applying a cut generation phase at the root node that adds cuts of either one of the three types, outperforms pure branch-and-bound. Finally, Wu et al. (1998) propose Tuy's cut for LP-LP problems but did not test it in a numerical study.

Very recently, a new valid inequality for LP-LP bilevel optimization based on strong duality of the lower-level problem has been presented in Kleinert, Labbé, et al. (2020a), which couples primal bilevel variables as well as dual variables of the lower-level problem:

$$\lambda^\top b - \lambda^\top C^+ - d^\top y \leq 0,$$

with C^+ being an upper bound on $C_i x$. For instance, the bounds C_i^+ can be computed with the auxiliary LPs

$$C_i^+ := \max_{x,y,\lambda} \{C_i x : (x, y, \lambda) \in H \times \{\lambda : D^\top \lambda = d, \lambda \geq 0\}, (x, y, \lambda) \in \mathcal{C}\},$$

where \mathcal{C} is a constraint set containing already added valid inequalities of any type as well as branching decisions or might be empty. While the inequality can be applied throughout the entire branch-and-bound tree, it is shown that it is most effective at the root node. In Kleinert and Schmidt (2020), it is shown that when equipping both approaches, the classical big- M approach and an SOS1-approach for the KKT complementarity conditions, with the root node inequality, then the two approaches perform very competitive—but the SOS1-approach does not suffer from the possible theoretical issues of invalid big- M values. The computational study in Kleinert and Schmidt (2020) is based on a LP-LP test set containing 1077 instances with up to

several thousands of upper- and lower-level variables and constraints. We note that the approaches tested in Kleinert and Schmidt (2020) are capable of solving 1051 out of the 1077 instances within a time limit of 1 h.

So far, most approaches discussed exploit the (structure of the) KKT reformulation (8) of the bilevel problem. On the other hand, there also exist approaches that are based on reformulation (10). The issues with this reformulation are the nonconvex bilinear terms involving primal upper- and dual lower-level variables. In principle, such nonconvex problems can be solved using classical convex envelopes—like those obtained using McCormick inequalities; see McCormick (1976). These convex envelopes can be refined by spatial branching to reduce the domain of the considered part of the nonconvex function. We refer the interested reader to Horst and Tuy (2013) for details and a convergence analysis of spatial branching methods in specific as well as for an overview of global optimization in general. Today, also general-purpose mixed-integer solvers such as Gurobi (Achterberg 2019) and CPLEX (Klotz 2017) can solve problems including these bilinear nonconvexities.

In bilevel optimization, very often the assumption is made that the linking variables, i.e., those upper-level variables that also appear in the lower-level constraints, are bounded integers. In this case, the bilinear terms $\lambda^\top Cx$ can be linearized if upper bounds on λ are available. Note, however, that finding these upper bounds is the same task as finding big- M values for the KKT reformulation. Nevertheless, if such a big- M is at hand, in Zare et al. (2019) it is shown that in case of large lower-level problems (measured in terms of the number of constraints), the strong-duality based reformulation (10) outperforms the KKT-based approach. The same assumption and linearization technique is used in Kleinert, Grimm, et al. (2020), where an outer approximation algorithm for MIQP-QP bilevel problems with convex-quadratic lower levels is presented.

Let us close this section with some brief pointers to local methods. Recently, classical MPCC regularization techniques such as the famous regularization proposed by Scholtes (2001) have been used to compute C-stationary solutions of the KKT reformulation in Dempe and Franke (2019). In Dempe (2019), even locally optimal solutions of the linear bilevel problem are obtained based on the KKT reformulation. Stationary points of (10) are computed in Kleinert and Schmidt (2019a) by using a penalty alternating direction method. The quality of this method as a primal heuristic for the bilevel problem at hand is evaluated in an extensive computational study. It demonstrates that the approach is capable of computing feasible points for large instances with thousands of variables and constraints, often in a fraction of a second. Related penalty methods for the linear bilevel problem are discussed in Anandalingam and White (1990), Campelo et al. (2000), and Lv et al. (2007).

Last but not last, let us refer to the recent survey chapter by Calvete and Galé (2020) on algorithms for linear bilevel problems.

4. BILINEAR LOWER LEVELS

A bilevel problem for which the lower level contains bilinearities but which is a linear problem when the upper-level variables x are fixed can also be reformulated as a single-level optimization problem by using any of the two techniques described in Section 3.2. Pricing problems and bimatrix Stackelberg games constitute two classes of bilevel problems that present this feature.

4.1. Pricing Problems. A first bilevel pricing problem with linear constraints, linear upper-level objective and bilinear lower-level objective has been proposed by Bialas and Karwan (1984). The following problem considered in Labbé, Marcotte,

et al. (1998) provides a general framework for pricing:

$$\max_{x, y=(y_1, y_2)} x^\top y_1 \quad (11a)$$

$$\text{s.t. } Ax \leq a, \quad (11b)$$

$$y \in \arg \min_{\bar{y}} \{(x + d_1)^\top \bar{y}_1 + d_2^\top \bar{y}_2 : D_1 \bar{y}_1 + D_2 \bar{y}_2 \geq b\}. \quad (11c)$$

The vector y of lower-level variables is partitioned into two sub-vectors y_1 and y_2 , called plans, that specify the levels of some activities such as goods or services. The upper level influences the activities from plan y_1 through a price vector x it charges to the lower level and maximizes its revenue given by $x^\top y_1$. The price vector x is subject to linear constraints that may, among others, impose lower and upper bounds on the prices. Vectors d_1 and d_2 represent linear disutilities faced by the lower level when executing the activity plans y_1 as well as y_2 . Note that d_2 may also encompass the price for executing the activities not influenced by the upper level. These activities may, e.g., be substitutes offered by competitors for which prices are known and fixed. The lower level determines its activity plans y_1 and y_2 to minimize the sum of total disutility and the price paid for plan y_1 subject to linear constraints. Remark that if the model allows negative prices then it implicitly permits subsidies, which may be appropriate, e.g., in the context of a central agency determining taxes. In order to avoid the situation in which the upper level would maximize its profit by setting prices to infinity for these activities y_1 that are essential, one may assume that the set $\{y_2 : D_2 y_2 \geq b\}$ is nonempty. Indeed, in this case, there exists a feasible point for the lower level that does not use any activity influenced by the upper level.

We now discuss some interesting geometrical properties of the bilevel pricing problem. First, remark that the feasible region of the lower level (11c) is independent of the upper-level variables x , which is in contrast to the lower level (7) of the LP-LP problem. Assuming that the feasible region of the lower level is bounded, i.e., a polytope, allows us to conclude that for every upper-level decision the optimal solution of the lower level is attained at a vertex of the feasible polytope of the lower level. In addition, strong duality holds for every parametric lower level problem (11c). Second, we look at the single-level reformulation of Problem (11) obtained by using the KKT conditions of the lower-level problem (11c):

$$\max_{x, y=(y_1, y_2), \lambda} x^\top y_1 \quad (12a)$$

$$\text{s.t. } Ax \leq a, \quad D_1 y_1 + D_2 y_2 \geq b, \quad (12b)$$

$$D_1^\top \lambda = x + d_1, \quad D_2^\top \lambda = d_2, \quad \lambda \geq 0, \quad (12c)$$

$$\lambda^\top (D_1 y_1 + D_2 y_2 - b) = 0. \quad (12d)$$

Let (\bar{y}_1, \bar{y}_2) be a fixed vertex of the feasible polytope of the lower level. Then, the constraints of (12) are linear in x and λ , i.e., they constitute a polyhedral set for fixed (\bar{y}_1, \bar{y}_2) . By considering all vertices of the lower level, we determine a partition of the feasible set of Problem (12) into a (possibly exponential) number of polyhedral cells with the property that all price vectors x belonging to a cell share the same lower-level optimal solution. Some of these cells may be empty. As a consequence, the objective function of the bilevel pricing problem is neither convex nor continuous in x but is linear in each cell.

Formulation (12) contains nonlinear terms both in its objective function (12a) and in constraints (12d). To circumvent the nonlinearity of the latter one might use the approach proposed by Fortuny-Amat and McCarl (1981) that is described in Section 3.3 but to do so, again one needs to bound the dual variables, which is NP-hard in general as mentioned earlier. Another approach consists of replacing

the complementarity constraints by the strong duality condition

$$(x + d_1)^\top y_1 + d_2^\top y_2 \leq b^\top \lambda.$$

that involve the same bilinear term as the objective function (12a). Grimm, Orlinkaya, et al. (2020) use the latter kind of reformulation for the lower-level problem for particular cases of the above bilevel pricing problem (11) that correspond to different electricity retailer pricing schemes. Zugno et al. (2013), on the other hand, consider a similar electricity pricing problem but use the KKT optimality conditions and the single-level reformulation à la Fortuny-Amat and McCarl (1981).

If all vertices of the feasible polytope of the lower level are binary, bilinear terms can be linearized more efficiently when using the approach proposed by McCormick (1976). This particularly applies to lower-level problems that are polynomial graph problems. Van Hoesel (2008) and Labbé and Violin (2013) present surveys about such so-called network pricing problems that we briefly sketch in the following. Consider a graph whose arc weights represent travel costs. In the toll setting problem, the upper level determines the prices (or tolls) of a subset of arcs of a network in order to maximize its revenue obtained by collecting tolls paid by the lower level that consists in a given number of users, each one being an independent follower. Each user selects a path from her origin to her destination that minimizes her disutility given by the sum of the prices of the arcs in the path that are controlled by the upper level plus the total travel costs.

Labbé, Marcotte, et al. (1998) show that the toll setting problem with (possibly negative) lower bounds on the prices is NP-hard even for a single user and that it is polynomial in the special case that one single arc is to be priced. Roch et al. (2005) strengthen the complexity result by showing that the single-user toll setting problem is already strongly NP-hard if all lower bounds on the prices are equal to 0. Joret (2011) shows that the problem is also APX-hard. Labbé, Marcotte, et al. (1998) propose a MILP reformulation of the toll setting problem that involves big- M values. Dewez et al. (2008) show how to derive efficient big- M s and propose valid inequalities that strengthen the MILP model. Brotcorne, Labbé, et al. (2001) propose heuristics and Bouhtou et al. (2007) present a preprocessing method to reduce the graph size. Didi-Biha et al. (2006) and Brotcorne, Cirinei, et al. (2011) exploit the fact that revenue maximizing prices that are compatible with a given lower-level solution can be easily determined. They propose exact algorithms as well as heuristics based on multi-path generation.

Heilporn et al. (2010b) and Heilporn et al. (2011) study the particular case in which each follower uses at most one arc priced by the leader. Heilporn et al. (2010b) show that the problem is strongly NP-hard. Further, exploiting the fact that there exists a limited number of feasible solutions for each follower, they provide an MILP formulation based on the optimal value function, a polyhedral study of this formulation, and provide a complete description of the convex hull of feasible points for the special case of one single follower. In Heilporn et al. (2011), a branch-and-cut procedure is proposed.

Heilporn et al. (2010a) show the equivalence of this problem with the so-called product line pricing problem. In the upper level of this problem, prices of products must be determined to maximize total revenue. In the lower level, customers choose the product that maximizes their welfare given by the difference of their reservation price (also called willingness to pay) for the product and its price. The product line design and pricing was originally introduced by Dobson and Kalish (1988). Guruswami et al. (2005) show that it is APX-hard. MILP formulations different than the one used in Heilporn et al. (2010b) are presented in Shioda et al. (2011), Myklebust et al. (2016), and Fernandes et al. (2016). Moreover, heuristics are proposed in Dobson and Kalish (1993), Shioda et al. (2011) as well as Myklebust et

al. (2016). Instance generators that are publicly available are described in Fernandes et al. (2016).

Castelli et al. (2017) show that the special case in which the price of all arcs controlled by the leader must be equal is polynomial. Furthermore, they also show that the problem is pseudo-polynomial when arc prices must be proportional to their length and they also consider a robust variant of these problems. Castelli et al. (2013) apply the model with proportional prices in the context of air traffic management to determine how much Air Navigation Service Providers (ANSPs) should charge airlines to use their airspace.

Marcotte, Mercier, et al. (2009) use the toll setting problem to determine road tolls to regulate the use of roads for hazardous shipments and show that an optimal toll policy is more efficient than a network design approach that determines road segments to be closed to dangerous materials.

Brotcorne, Labbé, et al. (2008) consider the more general problem in which the leader faces a joint design and pricing problem. Here, in the upper-level objective, a fixed cost is incurred for each arc that is installed (and priced) by the leader. The lower level is the same as in the toll setting problems. They show that the coupling constraints linking the design variables and the user arc choice variables appearing in the lower level can be moved to the upper level. These constraints forbid the followers to use arcs that are not installed. Moving them to the upper level is allowed because the leader can prevent the followers to use them by setting their price very high. Finally, they suggest a single-level MILP formulation as well as heuristics.

Network pricing problems with different lower-level problems have also been studied. Brotcorne, Labbé, et al. (2000) consider a lower level given by an uncapacitated transshipment problem and provide an MILP formulation as well as some heuristics. Another variant is obtained by assuming that the lower level selects a minimum spanning tree. Cardinal et al. (2011) show that this problem is APX-hard, whereas Morais et al. (2016) and Labbé, Pozo, et al. (2021) propose different MILP formulations.

4.2. Stackelberg Bimatrix Games. The determination of optimal mixed strategies in a Stackelberg bimatrix game under normal form constitutes another typical bilevel problem in which both objectives are bilinear (in both the upper- and lower-level variables) and all constraints are linear. In such a game, two players, say A and B are endowed with a set of pure strategies I and J with $|I| = n, |J| = m$. The matrices $R = [R_{ij}]$ and $C = [C_{ij}]$ encode the respective utilities when A plays strategy i and B plays strategy j . A mixed strategy for player A (B) is a probability distribution x (y) over her pure strategy set I (J). Both players want to maximize their respective expected utility given by $x^\top Ry$ and $x^\top Cy$. Now assume that the players choose their mixed strategy sequentially: A is the leader and plays first, then B, informed of A's decision, reacts optimally with respect to her own objective. The solution to this Stackelberg bimatrix game, called a Strong Stackelberg Equilibrium (SSE), is given by an optimal solution of the bilevel problem

$$\max_{x,y} x^\top Ry \quad (13a)$$

$$\text{s.t. } \mathbb{1}^\top x = 1, x \geq 0, \quad (13b)$$

$$y \in \arg \max_{\bar{y}} \{x^\top C\bar{y} : \mathbb{1}^\top \bar{y} = 1, \bar{y} \geq 0\}, \quad (13c)$$

in which $\mathbb{1}$ denotes the vector of all ones in appropriate dimension. The term "strong" stands for the fact that the optimistic version of the problem is considered. Conitzer and Sandholm (2006) describe and discuss different representations of such

leader-follower games as well as the appropriateness and the utility of using pure or mixed strategies. Furthermore, SSE's may not coincide with Nash equilibria, as shown by the example provided in Korzhlyk, Yin, et al. (2011).

Problem (13) can be solved using linear programming. First notice that for a given leader's solution x , the lower level is an LP on the unit simplex. In other words, there always exists an optimal solution for the follower that is one of the n vertices of the unit simplex. Second, a solution x that maximizes the leader's utility and for which some solution \bar{y} , with $\bar{y}_j = 1$ for some $j \in J$, is optimal for the follower can be found by solving problem (13) whose objective function is $x^\top R_{.j}$ and in which the lower-level problem (13c) is replaced with

$$x^\top C_{.j'} \leq x^\top C_{.j} \quad \text{for all } j' \in J.$$

Hence, solving this LP for every possible pure strategy of the follower and retaining the one that yields the highest utility for the leader provides an SSE; see Conitzer and Sandholm (2006).

Problem (13) can be adapted to the case in which the leader does not know the follower's preferences over the outcomes of the game with certainty. This is done by considering different types $k \in K$ of followers. In this case, the game is called Bayesian. Utility matrices R^k and C^k are then given for each follower type k as well as a probability π^k that the type of the follower is indeed k . The leader's expected utility is then equal to $\sum_{k \in K} \pi^k x^\top R^k y^k$ and a lower-level problem

$$y^k \in \arg \max_{\bar{y}^k} \{x^\top C^k \bar{y}^k : \mathbb{1}^\top \bar{y}^k = 1, \bar{y}^k \geq 0\}$$

is introduced for each follower type. A Bayesian Stackelberg bimatrix game can be seen as a regular Stackelberg bimatrix game in which the set of pure strategies of the follower is composed of all $n^{|K|}$ possible combined choices of pure strategies of the different follower types; see Harsanyi and Selten (1972). As a consequence, an SSE in a Bayesian Stackelberg bimatrix game can be determined in polynomial time when the number of types is fixed. If not, the problem is NP-hard; see again Conitzer and Sandholm (2006).

The bilevel optimization problem that determines an SSE of a general Bayesian Stackelberg bimatrix game can be reformulated as a single-level MILP. In fact any of the three approaches consisting in using KKT conditions, strong duality, or the optimal value function leads to an equivalent single-level reformulation. Then, to circumvent the bilinearities in the objective functions of both levels, one may exploit the fact that there always exists an optimal follower's response that is binary, i.e., it is a pure strategy. Paruchuri et al. (2008), Kiekintveld et al. (2009), and Yin and Tambe (2012) propose models based on these principles. The LP relaxation of the formulation proposed by Yin and Tambe (2012) is the strongest and provides a complete description of the convex hull of feasible points in the case of a single follower. See Casorrán et al. (2019) for comparison of the three above mentioned formulations from both theoretical and computational point of views. On the other hand, decomposition methods scale better when the problem involves many resources and/or follower types. In this perspective, Paruchuri et al. (2008) propose a solution approach involving Benders decomposition and Jain, Kardes, et al. (2010) and Lagos et al. (2017) use column generation.

Stackelberg bimatrix games have been shown to be useful for many real-world applications in security domains. In these so-called Stackelberg security games, the leader (defender) places security resources (e.g., guards) at various potential targets (possibly in a randomized manner), and then the follower (attacker) chooses a target to attack; see e.g. Jain, An, et al. (2013). Examples of such applications include disrupting drug trafficking networks (Washburn and Wood 1995), assigning Federal

Air Marshals to transatlantic flights (Pita, Jain, Marecki, et al. 2008), determining randomized port and waterways patrols for the U.S. Coast Guard (Shieh et al. 2012), preventing fare evasion in public transport systems (Yin, Jiang, et al. 2012), protecting endangered wildlife (Yang et al. 2014), or coordinating resources to organize patrols of the Chilean national police force (Bucarey et al. 2019). See also the book edited by Tambe (2011) that describes many applications and the survey by Sinha, Fang, et al. (2018) that presents recent advances in Stackelberg security games. In these security games, playing a mixed strategy of the defender is particularly appropriate because even if the attacker is aware of this mixed strategy, she does not know which pure strategy will actually be put in action when she attacks. This is especially relevant when the game is played in a repeated way, e.g., every day.

A common feature of Stackelberg security games is that pure strategies of the leader consist in allocating several resources to protect targets, leading to an exponential number of such pure strategies. In the simplest case, J represents a set of targets that may be attacked and each target attack corresponds to a pure strategy of the attacker. Further, assume that the defender has a set of $m < n$ (identical) resources available to cover these targets. The possible pure strategies of the defender consist in all subsets of J of cardinality at most m . As a consequence, any of the formulations proposed for finding an SSE in a general bimatrix Stackelberg game becomes rapidly intractable when the number of targets and/or resources increase.

To alleviate this situation, Kiekintveld et al. (2009) propose to encode a leader's mixed strategy by a vector x whose entries x_j represent the marginal probabilities of covering each target j in this mixed strategy. The marginal probability of a target is equal to the sum of the probabilities of the pure strategies covering the said target. In other words, a vector x of marginal probabilities is a point belonging to the convex hull of the binary vectors corresponding to all possible pure strategies, i.e., all binary vectors with at most m entries equal to 1. It can be readily seen that this convex hull is $\{x: \mathbb{1}^\top x \leq m, 0 \leq x \leq \mathbb{1}\}$. Indeed, the constraint matrix is totally unimodular so that all the vertices of this polytope are binary vectors. Further, as explained in Kiekintveld et al. (2009), the mixed strategy corresponding to a given vector of marginal probabilities can be retrieved in polynomial time since it amounts to solve a linear system with a polynomial number of constraints. In the context of a scheduling problem, McNaughton (1959) proposes an alternative and faster polynomial procedure.

Another common feature of Stackelberg security games is that the utility of both the defender and the attacker depend only on whether the target that is attacked is protected or not. There are two cases, depending on whether or not the target is covered by the defender. The defender's utility for an uncovered attack of type k on target j is denoted $D^k(j|u)$ and for a covered attack of type k it is denoted as $D^k(j|c)$. Similarly, $A^k(j|u)$ and $A^k(j|c)$ represent the type k attacker's utilities. With these new notations at hand, one can formulate the following bilevel problem that determines an SSE in a Bayesian Stackelberg security game:

$$\begin{aligned} \max_{x,y} \quad & \sum_{k \in K} \pi^k \sum_{j \in J} (x_j D^k(j|c) + (1 - x_j) D^k(j|u)) y_j^k \\ \text{s.t.} \quad & \mathbb{1}^\top x \leq m, 0 \leq x \leq \mathbb{1}, \\ & y^k \in \arg \max_{\bar{y}^k} \left\{ \sum_{j \in J} (x_j A^k(j|c) + (1 - x_j) A^k(j|u)) \bar{y}_j^k : \mathbb{1}^\top \bar{y} = 1, \bar{y} \geq 0 \right\}. \end{aligned}$$

Three single-level MILP reformulations similar to the ones proposed for general Stackelberg games can be derived for this problem; see Casorrán et al. (2019). The authors also compare them with extended formulations that involve all possible mixed strategies, i.e., formulations of the general Stackelberg game version of such security games.

Other variants of Stackelberg security games involve more sophisticated pure strategies of the leader. Resources can be heterogeneous meaning that each resource can only cover a subset of targets. Resources can cover at once a subset of targets, called schedule. Korzhyk, Conitzer, et al. (2010) investigate the complexity of such variants with one type of follower. They show that a Stackelberg security game with homogeneous resources is polynomial if the schedules have size at most 2 and is NP-hard otherwise. When resources are heterogeneous, they show that the problem is polynomial when schedules have size 1 and NP-hard otherwise. Jain, Kardes, et al. (2010) propose a branch-and-price approach for such variants by iteratively generating columns representing pure strategies of the leader. Finally, Letchford and Conitzer (2013) study the complexity of the case of Stackelberg security games in which the targets are vertices of a graph and schedules are subgraphs with a particular structure such as path or tree.

5. MIXED-INTEGER (NON)LINEAR LOWER LEVELS

In this section, we focus on a general bilevel MILPs, which are defined as

$$\min_{x \in X, y} c_x^\top x + c_y^\top y \quad (14a)$$

$$\text{s.t. } Ax + By \geq a, \quad (14b)$$

$$y \in \arg \min_{\bar{y} \in Y} \{d^\top \bar{y} : Cx + D\bar{y} \geq b\}, \quad (14c)$$

where the vectors c_x, c_y, d, a, b and matrices A, B, C, D are defined as in Section 3. The sets X and Y specify integrality constraints on a subset of x - and y -variables, respectively.

The HPR's feasible region of this bilevel MILP is, as usual, defined as the set of points $(x, y) \in X \times Y$ satisfying all constraints of the upper and lower level, i.e.,

$$H := \{(x, y) \in X \times Y : Ax + By \geq a, Cx + Dy \geq b\}.$$

The inducible region of a bilevel MILP consists of all bilevel feasible points, i.e., all points $(x, y) \in H$ for which for a given x , the vector y is an optimal solution of the lower-level problem. This means,

$$d^\top y \leq \varphi(x),$$

holds. Here, $\varphi(x)$ again is the optimal value of the lower-level problem, which is defined as

$$\varphi(x) = \min_{y \in Y} \{d^\top y : Dy \geq b - Cx\}. \quad (15)$$

The value function $\varphi(x)$ thus corresponds to a parametric MILP, and hence it is nonconvex, not continuous, and in general very difficult to describe. Moreover, in contrast to bilevel LPs, it is NP-hard to check whether a given point (x, y) is a feasible solution of the bilevel MILP. Jeroslow (1985) showed that k -level discrete optimization problems are Σ_k^P -hard, even when the variables are binary and all constraints are linear. This means that, e.g., a discrete bilevel optimization problem can be solved in nondeterministic polynomial time, provided that there exists an oracle that solves problems that are in NP in constant time.

The inducible region of the bilevel MILP is contained in the set H , and therefore, minimizing the objective function of the upper level over the set H (which represents

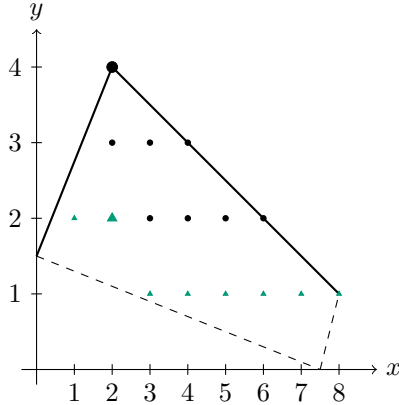


FIGURE 2. Example of a bilevel MILP: Discrete points are feasible for the high-point relaxation. The point $(2, 4)$ is the optimal solution of the high-point relaxation and $(2, 2)$ is the optimal solution of the bilevel MILP. Triangles represent bilevel feasible solutions and dashed lines represent the feasible region of the bilevel LP in which the integrality constraints on the upper- and lower-level variables are relaxed.

another MILP) provides a valid lower bound for the bilevel MILP. Consequently, solving the LP-relaxation of the HPR provides another (and usually much weaker) lower bound of the bilevel MILP.

Moore and Bard (1990) initiated the studies of bilevel optimization problems involving discrete variables. Their illustrative example (cf. Figure 2) is frequently used in the literature to highlight the major differences and pitfalls arising in discrete bilevel optimization. Since then, studies have been carried out considering only special cases, e.g., by assuming binary variables at both levels or by considering purely linear problems at the lower level. Exact MILP-based procedures for the general case in which both the upper and the lower level are MILPs have been mainly studied in the last decade.

5.1. General Properties. The following example is provided by Moore and Bard (1990):

$$\min_{x \in \mathbb{Z}, y \in \mathbb{Z}} \left\{ -x - 10y : y \in \arg \min_{\bar{y} \in \mathbb{Z}} \{ \bar{y} : (x, \bar{y}) \in \mathcal{P} \} \right\},$$

where \mathcal{P} is a polytope defined by

$$-25x + 20\bar{y} \leq 30, \quad x + 2\bar{y} \leq 10, \quad 2x - \bar{y} \leq 15, \quad 2x + 10\bar{y} \geq 15.$$

The HPR of this problem is an integer linear problem, whose feasible region is depicted in Figure 2. The unique optimal solution for this example is the point $(2, 2)$, which is in the interior of the convex hull of the HPR. This is in contrast to bilevel LPs, whose optimal solution is always a vertex of the HPR; see Section 3. The example also shows that relaxing the integrality constraints for the lower-level problem does not provide neither lower nor upper bounds for the bilevel MILP. Dashed lines in Figure 2 correspond to the inducible region of the problem in which the integrality constraints for both the upper-level and the lower-level variables are relaxed. In general, such obtained set does not even have to contain a single bilevel feasible point.

For a general study of representability of sets by extended formulations using mixed-integer bilevel programs we refer to the recent paper by Basu et al. (2021).

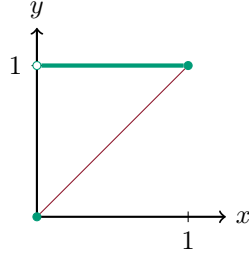


FIGURE 3. The attainability counterexample by Köppe et al. (2010)

Attainability of Optimal Solutions. In Vicente, Savard, et al. (1996), the authors consider three cases of bilevel MILPs and study the following different assumptions:

- (i) only upper-level variables are discrete,
- (ii) all upper- and lower-level variables are discrete, and
- (iii) only lower-level variables can take discrete values.

Assuming that all discrete variables are bounded and that the inducible region is nonempty, they show that for Case (i) and (ii), an optimal solution always exists and that (i) can be reduced to a linear bilevel program (cf. Section 3), whereas (ii) can be reduced to a linear trilevel problem. However, for Case (iii), Moore and Bard (1990) and also Vicente, Savard, et al. (1996) provided examples that demonstrate that the bilevel feasible region may not be closed, and hence, the optimal solution may not be attainable. The following simpler example (see Figure 3) is due to Köppe et al. (2010):

$$\inf_{0 \leq x \leq 1, y} \left\{ x - y : y \in \arg \min_{y' \in \mathbb{Z}} \{ \bar{y} : \bar{y} \geq x, 0 \leq \bar{y} \leq 1 \} \right\},$$

which is equivalent to

$$\inf_x \{ x - \lceil x \rceil : 0 \leq x \leq 1 \}.$$

In this problem, the infimum is -1, which is never attained. In the existing literature on bilevel MILPs, it is therefore frequently assumed that the linking variables are discrete. We recall that nonlinking upper level variables can be moved to the lower level (Bolusani and Ralphs 2020; Tahernejad et al. 2020), which effectively translates the latter assumption into “all upper-level variables are discrete”. Alternatively, for bilevel MILPs with continuous linking variables, methods that achieve ε -optimal solutions are considered if the optimal solution cannot be attained; see, e.g., Zeng and An (2014). Fanghänel and Dempe (2009) analyzed the structure of bilevel MILPs with continuous upper-level and discrete lower-level variables. They also discussed optimality conditions for local and global optimality.

Unboundedness of the Lower-Level Problem. A common assumption for algorithms dealing with bilevel MILPs is that the feasible region of the HPR is compact. Sometimes, this condition is relaxed and it is only assumed that discrete variables are bounded. For the latter case, Xu and Wang (2014) demonstrate that the unboundedness of the optimal HPR value does not reveal the nature of the underlying bilevel problem. It can happen that the underlying bilevel MILP is infeasible, unbounded, or admits an optimal solution; see also Section 3 for an illustrative example. Xu and Wang (2014) (cf. Lemma 2) also show that if the lower level MILP (15) is unbounded (i.e., $\varphi(x) = -\infty$ for a certain x from the HPR’s feasible region), then the bilevel MILP (14) is infeasible. Later, Fischetti, Ljubić, et al. (2018) showed that for any bilevel MILP whose HPR value is unbounded,

one can detect upfront whether the lower-level problem is unbounded or not. To this end, it is sufficient to solve a single LP (not depending on x) in a presolve phase. The solution of this LP, cf. Theorem 1 of Fischetti, Ljubić, et al. (2018), provides a direction (if such exists) in which the lower-level problem defined by (15) is unbounded—no matter the choice of the vector x from the HPR’s feasible region.

5.2. Generic Approaches for Bilevel MILPs. Most of the exact methods studied in the literature start with solving the high-point relaxation, i.e., $\min\{c_x^\top x + c_y^\top y: (x, y) \in H\}$, and continue by discarding bilevel infeasible solutions by branching, by adding cutting planes, by approximating the value function $\varphi(x)$ given in (15), or by a combination of all of them. In the following, we review these methods and point out to their differences.

Branch-and-Bound Methods. In their seminal paper, Moore and Bard (1990) develop the first branch-and-bound method for discrete bilevel optimization. Their algorithm terminates after a finite number of iterations if all upper-level variables are integer or all lower-level variables are continuous (assuming an optimum exists). In addition, the authors assume that the HPR’s feasible region is compact and that there are no coupling constraints at the upper level. The authors point out that two of the three standard B&B fathoming rules for mixed-integer optimization are not valid in the bilevel context and discuss further computational challenges of solving discrete bilevel problems. Bard and Moore (1992) then propose another exact algorithm for bilevel MILPs assuming that all variables (x, y) are binary.

Fischetti, Ljubić, et al. (2018) developed another branch-and-bound method that works for mixed-integer upper- and lower-level problems and allows coupling constraints at the upper level. The major assumption is that the discrete variables are bounded and that the linking variables are discrete. Necessary modifications of a standard B&B-based MILP solver are introduced to properly handle branching, node evaluation, and fathoming rules. The method checks unboundedness of the lower-level problem in a presolve phase; see Section 5.1. Together with Xu and Wang (2014), see below, the proposed B&B algorithm is one of the few methods that return a provably optimal solution (if such exists) within a finite number of iterations without assuming that the HPR’s feasible region is compact. Instead, only the discrete variables need to be bounded.

Parametric Integer Programming Methods. Faísca et al. (2007) assume that discrete variables of the bilevel MILP are binary and use parametric programming to develop an exact method that works in two phases. In the first phase, all K lower-level solutions are enumerated using parametric integer programming. Then, each solution is plugged into the upper-level problem, yielding K single-level MILP problem reformulations, from which the best one represents the global optimum. The approach is picked up and extended to bilevel MIQPs in Avraamidou and Pistikopoulos (2019a). The authors also provide a computational study for bilevel MILPs and bilevel MIQPs. A more detailed description of the implementation can be found in Avraamidou and Pistikopoulos (2019b).

Köppe et al. (2010) also approach bilevel MILPs from the parametric programming perspective. They view the lower-level problem as a parametric (integer) program whose right-hand side is parameterized by x . The authors propose an algorithm that runs in polynomial time for a fixed dimension n_y of the lower-level problem and for the case that the linking variables are continuous. In case the linking variables are discrete, the authors show that there exists an algorithm that runs in polynomial time for a fixed dimension $n_x + n_y$. The algorithm applies binary search by targeting the optimal value of the bilevel MILP.

Multi-Way Branching. Xu and Wang (2014), see also the PhD thesis by Xu (2012), apply a multi-way branching method to solve bilevel MILPs in which all leader variables are required to be integer and bounded. The algorithm solves a series of MILPs obtained by restricting the values of slack variables of the lower-level constraints. Another enhanced version of this method, which provides a heuristic solution in the case that the lower-level problem has multiple optimal solutions, is given by Liu, Wang, et al. (2020).

In their “watermelon algorithm”, Wang and Xu (2017) exploit multi-way branching to “carve out” bilevel infeasible points from the feasible region of the HPR. Whenever a bilevel infeasible point (together with a polyhedron around it that contains no bilevel feasible points) is discovered, it is discarded by decomposing the search space into a family of smaller polyhedra, which are then solved in a recursive fashion. Two different ways to determine the bilevel-free polyhedron around a given infeasible point are proposed along with MILP-based procedures for their determination.

Branch-and-Cut Methods. By extending the ideas from Moore and Bard (1990), DeNegre and Ralphs (2009), see also the dissertation by DeNegre (2011), develop an MILP-based branch-and-cut approach. Their method does not allow for any continuous variables and coupling constraints at the upper level. It is also assumed that all coefficients in the upper- and lower-level constraints are integer. Bilevel infeasible solutions are cut off on the fly by adding “integer no-good cuts” that exploit the integrality property of the upper- and lower-level variables. These cuts are guaranteed to separate bilevel infeasible points from the convex hull of the bilevel feasible region.

An extension of the former method that allows for a mixed-integer setting at both levels is given by Tahernejad et al. (2020). In this setting, “generalized no-good cuts” are used to remove all solutions for which the linking variables have a certain fixed value, and thus no integrality of the coefficients in the constraint matrices is required. The authors provide a comprehensive implementation that integrates many computational and algorithmic features proposed in the recent literature on bilevel MILPs.

A cutting plane method for bilevel MILPs in which all variables are discrete (and all coefficients at the upper- and lower-level are integer) is given by Caramia and Mari (2015). The authors solve the HPR and utilize a variant of “no-good” constraints (involving big- M s and ℓ_∞ -norms) to cut off nonoptimal responses from the follower on the fly. They also propose a B&C method with a specific branching rule derived from rounding the value of the optimal follower’s response.

Dempe and Kue (2017) consider two special cases of bilevel MILPs: (i) both levels contain discrete variables only and the leader influences the objective of the follower (i.e., the objective function is bilinear), and (ii) only the lower level contains discrete variables and the leader influences the right-hand-side of the follower. For the former case, the authors propose a B&C algorithm based on covering-type valid inequalities. For the latter case, the authors exploit the structural properties of the value function and derive an iterative MILP-based procedure in which the value function is refined. The methods have been illustrated on two small examples.

To enhance the performance of their basic B&B method, Fischetti, Ljubić, et al. (2018) introduce intersection cuts to separate integer bilevel infeasible points, thus obtaining a B&C approach for bilevel MILPs. These cuts, which are traditionally used for mixed-integer programming (see, e.g., Balas (1971)) are used here for the first time to solve bilevel MILPs: LP-optimal solutions (being integer but bilevel infeasible) are cut off by deriving a cut in which the LP-cone of this solution is intersected with a convex set that contains no bilevel feasible points. These cuts can be derived under the assumption that d and $Cx + Dy - b$ are integer for

any $(x, y) \in H$. In a follow-up article, Fischetti, Ljubić, et al. (2017a) provide additional computational techniques to further improve their B&C method. These techniques include new ways to derive intersection cuts, follower upper-bound cuts and variable fixing based on the properties of the lower-level problem. The results also include hypercube intersection cuts, which can deal with lower levels with continuous variables (and thus do not require any additional assumptions regarding the coefficients of the lower-level problem). The authors conducted a computational study on a set of 874 benchmark instances and reported optimal solutions for 822 of them. The code of Fischetti, Ljubić, et al. (2017a) is publicly available (Fischetti, Ljubić, et al. 2017b), and represents the current state-of-the-art exact method for general bilevel MILPs. The code is integrated within the commercial solver CPLEX. An alternative open-source implementation that includes features of Fischetti, Ljubić, et al. (2017a), but also many additional ones, has been developed by Tahernejad et al. (2020) and is available online (Ralphs 2018). Unsurprisingly, specialized approaches for solving particular interdiction problems, like those of Fischetti, Ljubić, et al. (2019) and Furini, Ljubić, San Segundo, and Zhao (2020), are outperforming the generic approaches by Fischetti, Ljubić, et al. (2017a) and Tahernejad et al. (2020) on interdiction instances.

Benders-like Decomposition. A Benders-like decomposition scheme for general bilevel MILPs is given in Saharidis and Ierapetritou (2009), assuming that the HPR’s feasible region is compact. Valid Benders-like cuts are derived by fixing the value of integer variables at the master level and using the active-set strategy together with the KKT reformulation of the resulting continuous lower-level problem. The algorithm terminates when an ε -optimal solution is achieved.

In a recent article by Bolusani, Coniglio, et al. (2020), the authors make a parallel between bilevel MILPs and two-stage stochastic MILPs with recourse. By exploiting their common mathematical structure given by the value-function reformulation and using the MILP-duality theory, a unified algorithmic framework is provided. In Bolusani and Ralphs (2020), a Benders-like decomposition to approximate the value function and a cutting-plane method are discussed as two possible solution strategies.

Other Approaches. Zeng and An (2014) proposed a single-level reformulation and a decomposition algorithm based on a column-and-constraint generation scheme for general bilevel MILPs. The authors even allow the linking variables of the leader to be continuous. Under the assumption that the optimal solution is attainable, the algorithm finds an optimal solution. Otherwise, it finds an ε -solution. Their idea is picked up by Yue, Gao, et al. (2019) who propose to project out integer variables of the lower-level problem and work with KKT conditions of the remaining continuous lower-level problem.

Another alternative approach for binary lower-level problems is recently proposed by Shi et al. (2020). The authors consider bilevel MILPs in which the lower-level variables are all binary. The method is based on the k -optimality of the lower-level solution: It is a relaxation of the lower-level problem in which the follower’s response is accepted by the leader as long as it is within the k -Hamming distance neighborhood of any bilevel feasible solution. This way, it is possible to model not completely rational decisions of the follower. The authors provide a hierarchy of decisions linked with the value of k , along with a hierarchy of upper and lower bounds of the original bilevel problem, which corresponds to $k = 0$.

5.3. Bilevel MINLPs. For single-level nonconvex mixed-integer optimization problems, one can only expect to compute ε -optimal solutions. Thus, the same also holds for nonconvex mixed-integer bilevel problems. We refer to Definition 3 in

Mitsos, Lemonidis, et al. (2008) for a formal definition of ε -optimality in the bilevel context and discuss some approaches for bilevel problems with general nonconvex mixed-integer lower-level problems in the following.

In Mitsos (2010), general bilevel MINLPs with continuity assumptions on all functions are considered. In addition, all variables are assumed to be bounded. The stated approach is an extension of the method proposed in Mitsos, Lemonidis, et al. (2008) that dealt with purely continuous bilevel problems. In turn, the latter paper builds on theoretical developments in Mitsos and Barton (2006). The key idea is to exploit estimates on the optimal value function of the lower level, which requires the global solution of MINLPs as subproblems. The approach is shown to terminate in finite time and an implementation of the approach is evaluated on a small test set.

In a series of papers, the so-called branch-and-sandwich approach for bilevel MINLPs is developed. The main idea is to subsequently compute tightened bounds on the optimal value function (3) and on the upper-level objective function value. Starting with continuous but nonconvex lower-level problems in Kleniati and Adjiman (2014b) and a numerical evaluation thereof in Kleniati and Adjiman (2014a), the approach is extended to the mixed-integer case in Kleniati and Adjiman (2015). The approach stated in the latter paper is applicable to problems with twice continuously differentiable functions F , f , G , and g and requires bounds on all variables. In this setting, the branch-and-sandwich approach terminates in finite time. Recently, novel bounding schemes for this approach have been published in Paulavičius and Adjiman (2020) and further implementation details can be found in Paulavičius, Gao, et al. (2020). Due to the general hardness of the problems under consideration, the computational study in Kleniati and Adjiman (2015) deals with rather small problems with up to 12 variables and 7 constraints.

A different setting is considered in Lozano and Smith (2017a). All functions F , f , G , and g are continuous but possibly nonconvex. In addition, the constraint functions G and g need to be separable in x and y , i.e., they have to be of the form $G(x, y) = G_1(x) + G_2(y)$ and $g(x, y) = g_1(x) + g_2(y)$. Under the assumptions that (i) the upper- and lower-level feasible regions are compact, (ii) $g_1(x)$ is integer-valued for all x , and (iii) all upper-level variables x are integers, the authors derive a finite solution approach based on the value-function reformulation (4). In particular, this approach is also capable of solving the pessimistic variant.

6. INTERDICTION PROBLEMS

Interdiction games are a special class of bilevel problems that aim at monitoring or halting an adversary's activity in a given environment. They are used to model defender-attacker settings in which the attacker (the follower) optimizes some objective such as a shortest path or a maximum flow in a network (see, e.g., Israeli and Wood (2002)), or maximizes the profit of the items that can be packed in a knapsack (Caprara et al. 2014; Fischetti, Ljubić, et al. 2019). The defender, who acts as the leader, has limited resources to protect the environment, e.g., by disabling the vertices/edges in a network or by changing their capacity, or by removing the knapsack items, to achieve the worst possible outcome for the attacker. Besides military applications, interdiction problems are extremely important in controlling the spread of infectious diseases (Assimakopoulos 1987; Furini, Ljubić, Malaguti, et al. 2021; Shen, Smith, and Goli 2012), spread of fake news in social networks (Baggio et al. 2021), in counter-terrorism and in monitoring of communication networks (Wang, Yin, et al. 2016).

Interdiction problems follow the common structure of bilevel problems without coupling constraints,

$$\min_{x \in X, y \in S(x)} \{F(x, y) : G(x) \geq 0\},$$

where constraints $G(x)$ describe some restrictions on the solution of the leader, typically including some budget or resource constraints, and $S(x)$ represents the set of optimal solutions of the x -parameterized lower-level problem. Interdiction problems model zero-sum Stackelberg games, i.e., they correspond to a competitive setting in which the leader and the follower have diametrically opposed objective functions:

$$F(x, y) = -f(x, y).$$

This is why interdiction problems can be alternatively stated as

$$\min_{x \in X} \{\varphi(x) : G(x) \geq 0\}, \quad (16)$$

where the follower's problem is stated in its maximization form:

$$\varphi(x) = \max_{y \in Y} \{f(x, y) : g(x, y) \geq 0\}. \quad (17)$$

The leader prevents certain activities of the follower by reducing the availability of some objects or resources—for example, items or nodes/edges in a network. Based on the relationships between the functions f and g and the nature of the leader's variables x , we make the following distinction.

Discrete Interdiction. In the discrete interdiction setting given below, the linking variables x_i are binary, and they are set to one if and only if the respective object i is unavailable for the follower. Thus, the objective function $f(x, y) = d^\top y$ is typically linear and the constraints $g(x, y) \geq 0$ in (17) are replaced by:

$$y_i \leq U_i(1 - x_i), \quad i \in N_x, \quad (18a)$$

$$\tilde{g}(y) \geq 0, \quad (18b)$$

where U_i represents the default upper bound for the follower variable y_i (modeling the availability of object i at the lower level), $N_x \subseteq \{1, \dots, n_x\}$ is the index set of the binary linking variables of the leader, and $\tilde{g} : \mathbb{R}^{n_y} \rightarrow \mathbb{R}^\ell$ are constraints that impose further restrictions on the follower's solution. To simplify the exposition, in the remainder of this section we assume that $n_y = |N_x|$.

Continuous Interdiction. In the continuous interdiction setting, the linking variables x_i are continuous (i.e., $0 \leq x_i \leq 1$ for $i \in N_x$) and they model a continuous increase of costs (or reduction of available capacities) imposed on the interdicted objects. For example, in max-flow interdiction settings, the leader is given a limited budget to reduce the available capacity of arcs/vertices, while the follower tries to maximize the flow in the resulting network; see, e.g., Lim and Smith (2007) and Wood (1993) and the further references therein. Alternatively, in the shortest-path interdiction (see, e.g., Israeli and Wood (2002)), the leader can increase the cost of arcs traversed by the follower and in this case, the constraints $g(x, y) \geq 0$ in (17) are replaced by $\tilde{g}(y) \geq 0$ and the objective function of the follower $f(x, y)$ becomes bilinear, i.e.,

$$f(x, y) = \sum_{i \in N_x} y_i(d_i + \delta_i x_i), \quad (19)$$

as it now encodes the increase of arc costs (modeled by δ) caused by the leader. Finally, one can also consider discrete interdiction problems with bilinear objective functions.

By the nature of the objective function, there is no distinction between optimistic and pessimistic solutions. It is also commonly assumed that the available budget of the leader is limited, so that the follower's problem (17) stays feasible.

In some very special cases, when the interdiction problem can be modeled as a bilevel LP, the problem is polynomially solvable; see, e.g., Fulkerson and Harding (1977), where it is shown that continuous interdiction of the shortest-path problem

can be equivalently stated as a minimum cost flow problem. However, discrete interdiction of the shortest-path problem in which the leader chooses k arcs to interdict (i.e., $G(x) \geq 0$ translates into $\mathbb{1}^\top x \leq k$), already is NP-hard (Ball et al. 1989). The latter problem is frequently referred to as the k -most-vital arcs problem. Just like for general bilevel MILPs, if the follower solves an NP-hard problem (e.g., the maximum knapsack problem or the maximum clique problem), the corresponding interdiction problem turns out to be Σ_2^P -hard (Caprara et al. 2014; Rutenburg 1994).

6.1. Commonly Studied Interdiction Problems. We provide below a classification of interdiction problems based on the structures of the encompassed lower-level problems.

Network Interdiction with Polynomial Lower-Level Problems. These problems model some of the most traditional and oldest applications arising in the areas of military or homeland security. Besides interdiction of shortest paths (Israeli and Wood 2002) or maximum flows (Akgün et al. 2011; Cormican et al. 1998; Janjarassuk and Linderoth 2008; Wood 1993), problems also have been studied in which the follower solves the spanning tree (Bazgan, Toubaline, and Vanderpooten 2013; Lin and Chern 1993) or the maximum matching problem (Zenklusen 2010).

Mixed-Integer Linear System Interdiction Problems. These are interdiction problems in which the lower level is an MILP. They were first studied in the PhD thesis of Israeli (1999) and later in the PhD thesis of DeNegre (2011). One of the most studied (and structurally easiest) variants is discrete interdiction of the maximum knapsack problem, in which the leader and the follower have a knapsack of their own, and the follower can only choose from those items that are not taken by the leader. Complexity results for this problem are given in Caprara et al. (2014), whereas tailored exact methods have been developed in Caprara et al. (2016), Della Croce and Scatamacchia (2019), and Fischetti, Ljubić, et al. (2019); see also PhD thesis by Carvalho (2016). The problem’s extension in which the leader and the follower solve a multidimensional knapsack problem has been addressed in Fischetti, Ljubić, et al. (2019). For other variants of more general bilevel knapsack problems (that do not belong to the interdiction setting) see the PhD thesis by Carvalho (2016) and the further references therein.

Facility location with interdiction has been studied as well. Scaparra and Church (2008) investigate the problem in which the leader is concerned with protecting a limited number of facilities, assuming the follower will attack a fixed number of them in order to maximize the transportation cost between the clients and the remaining operational facilities. In Zhang et al. (2016), the leader locates a fixed number of facilities first, followed by the follower, who is prohibited to use the same location as the leader. Both players face disruption risks while trying to maximize the market share, assuming that each customer patronizes the nearest open facility.

Interdiction problems on networks in which the follower solves an NP-hard problem also fall into this category. These problems include interdiction of the clique number (Furini, Ljubić, San Segundo, and Martin 2019; Furini, Ljubić, San Segundo, and Zhao 2020; Rutenburg 1994), or interdiction of independent sets and vertex covers (Bazgan, Toubaline, and Tuza 2011).

Blocking Problems. Closely related to interdiction problems are the so-called blocking problems in which the leader wishes to minimize the cost of blocking the activities of the follower, while ensuring the optimal follower’s response will be bounded by a user-defined threshold $r \in \mathbb{R}$:

$$\min_{x \in X} \{c_x^\top x : \varphi(x) \leq r, G(x) \geq 0\}.$$

When blocking the maximum number of cliques, e.g., the leader minimizes the (un)weighted sum of vertices/edges to remove from the graph, so that the maximum (weighted) clique in the remaining graph is bounded from above by a given integer (Pajouh 2020; Pajouh, Boginski, et al. 2014). The blocking of vertices or edges has been studied with respect to other graph optimization problems such as the maximum matchings (Zenklusen et al. 2009), shortest paths (Golden 1978), spanning trees (Bazgan, Toubaline, and Vanderpooten 2013), or dominating sets (Pajouh, Walteros, et al. 2015).

Most exact methods for blocker problems share similarities with the methods derived for interdiction problems, which is why we focus on the latter ones in the remainder of this section.

6.2. Methods. The specific structure of interdiction problems can be exploited in different ways to derive problem-tailored exact approaches. We summarize generic strategies used to solve interdiction problems to optimality.

Dualization. When the follower’s problem corresponds to a linear optimization problem, duality theory can be exploited to derive a single-level reformulation. If the leader influences the objective function of the follower, like in the bilinear objective function (19), we first dualize the lower-level problem for a given value of x . That way, we get rid of the bilinear terms and obtain a single-level formulation (see, e.g., Israeli and Wood (2002) for the shortest path interdiction) involving variables x of the leader and dual variables associated to constraints of the follower’s problem (17).

If the feasible region of the lower level is influenced by the leader, such as in (18), after dualizing the lower-level problem, the resulting single-level reformulation again optimizes over x and dual variables associated to each constraint of the follower’s problem. However, its objective function involves bilinear terms in which x -variables are multiplied with continuous variables of the follower’s dual problem. When dealing with discrete interdiction problems, these bilinear terms are typically linearized using McCormick’s inequalities (McCormick 1976), resulting in a single-level MILP problem reformulation; see, e.g., the seminal work by Wood (1993) where this technique is applied for the maximum-flow interdiction problem. For continuous x -variables, a specialized exact method has been proposed by Lim and Smith (2007) assuming that $G(x) \geq 0$ models a budget constraint, exploiting the fact that at most one of the x -components will be fractional in an optimal interdiction strategy.

Penalization. An alternative way to deal with constraints of type (18a) in a discrete interdiction setting is to relax them into

$$y_i \leq U_i, \quad i \in N_x, \quad (20)$$

and penalize the use of the object i , whenever $x_i = 1$ for an $i \in N_x$. This can be achieved by introducing coefficients M_i , $i \in N_x$, and by replacing the linear objective function $d^\top y$ of the follower by

$$\sum_{i \in N_x} y_i (d_i - M_i x_i).$$

Due to the fact that $x_i \in \{0, 1\}$, the coefficients M_i have to be sufficiently large to ensure that there always exists an optimal solution of the modified follower’s problem in which $x_i = 1$ implies $y_i = 0$ for all $i \in N_x$; see, e.g., Smith and Song (2020) and Wood (2011) and further references therein.

When the lower-level problem is linear, this transformation allows one to use duality theory and reformulate the problem as a single-level problem, following the same approach as for the bilinear objective function (19) described above. If

the lower-level problem is discrete (and NP-hard), one can apply a Benders-like decomposition approach instead.

Benders-like Decomposition. For linear lower-level problems, the value of M_i in the penalization approach is chosen as an upper bound of the dual variable associated to constraint (18a); see, e.g., Brown et al. (2006), Lim and Smith (2007), and Wood (2011).

Israeli (1999) proposes to use the penalty function to reformulate interdiction problems whose lower-level problem is an MILP. The lower-level problem is then convexified using the fact that its feasible region does not depend on x anymore and, hence, the value function can be restated as

$$\varphi(x) = \max \left\{ \sum_{i \in N_x} \bar{y}_i (d_i - M_i x_i) : \bar{y} \in \bar{Y} \right\}, \quad (21)$$

where \bar{Y} represents the set of extreme points of the polytope described by (18b) and (20). Recall that we assume that the lower-level problem is well defined, so that the set \bar{Y} is nonempty. Hence, the function $\varphi(x)$, described as the maximum of a set of affine functions given in (21), is convex and the starting problem, given in the Form (16), can be now reformulated by projecting out the follower's variables y and by introducing an auxiliary variable θ as

$$\min_{x \in X} \left\{ \theta : \theta \geq \sum_{i \in N_x} \bar{y}_i (d_i - M_i x_i), \bar{y} \in \bar{Y}, G(x) \geq 0 \right\}. \quad (22)$$

Recall that when the follower solves an NP-hard problem, the resulting interdiction problems are typically Σ_2^p -hard, which implies that there is no way of formulating such problems as single-level integer programs of polynomial size unless the polynomial hierarchy collapses. This, in particular, means that separating Benders-like constraints

$$\theta \geq \sum_{i \in N_x} \bar{y}_i (d_i - M_i x_i) \quad (23)$$

in (22) for any given solution $(\bar{\theta}, \bar{x})$ of the leader requires solving the NP-hard follower's problem defined by $\varphi(\bar{x})$ in (21). Nevertheless, when effective algorithms are available for solving these lower-level problems (rather than formulating them as MILPs and using general-purpose solvers), some recent results show that tight canonical single-level reformulations can be obtained. Fischetti, Ljubić, et al. (2019) use dynamic programming for the maximum knapsack interdiction and Furini, Ljubić, San Segundo, and Martin (2019) and Furini, Ljubić, San Segundo, and Zhao (2020) use tailored branch-and-bound solvers for two variants of the maximum clique interdiction problems. Moreover, any heuristic solution of the lower-level problem also provides a valid Benders-like constraint (23) and standard stabilization techniques for improving the convergence can be applied.

The choice of the coefficients M_i is crucial for the computational efficiency of the derived single-level reformulation. In some particular cases in which the follower solves an LP, such bounds can be very tight—for example, Cormican et al. (1998) show that $M_i = 1$ for the interdiction of the maximum flow problem. Recently, Fischetti, Ljubić, et al. (2019) show that tight M_i coefficients (i.e., $M_i = d_i$ for $i \in N_x$) can also be derived for lower-level problems which are NP-hard, provided that lower-level constraints satisfy the so-called downward monotonicity property. The latter property assumes that if \bar{y} is a feasible lower-level solution for a given x , then any \hat{y} such that $0 \leq \hat{y} \leq \bar{y}$ is also feasible. This condition is, for example, satisfied if the follower solves a variant of a set-packing problem (Dinitz and Gupta 2013), including the maximum knapsack, multidimensional knapsack, or

a graph optimization problem that satisfies the hereditary property with respect to interdicted objects; e.g., the maximum matching problem if edges are interdicted or the maximum clique problem if vertices are interdicted. Furini, Ljubić, San Segundo, and Martin (2019) show that for the maximum clique interdiction problem in which the leader removes the vertices of the graph, Constraints (23) are facet-defining with $M_i = 1$ under some mild conditions. Finally, Fischetti, Ljubić, et al. (2019) provide further generalizations of their result that include settings in which the follower’s MILP is an extended formulation, involving other variables that are not influenced by the leader (i.e., $n_y > |N_x|$) showing that interdiction of some facility location problems and variants of the Steiner tree problem fall into this category.

Other Approaches. Tang et al. (2016) propose a generic exact method for solving discrete interdiction problems in which the feasible region of the lower-level MILP is influenced by the leader. The authors show that valid lower bounds are obtained by progressively building a convex inner approximation of the feasible solutions of the lower-level MILP. This inner approximation is modeled as an LP, and dualized to obtain a single-level MILP formulation. The solution of this formulation provides a valid lower bound and a feasible solution x for the leader, which can be plugged in into $\varphi(x)$ to calculate a valid upper bound. The algorithm terminates when the lower and upper bound coincide or when all feasible solutions from $\{x \in X : G(x) \geq 0\}$ have been exhaustively searched.

Salmeron, Wood, and Baldick (2009) propose a global Benders decomposition method for discrete interdiction problems. The method alternates between solving the master problem (containing discrete interdiction variables) and LP subproblem(s), building a convex piecewise-linear approximation of the function $\varphi(x)$. The method is more general in the sense that it can be applied to interdiction problems for which the function $\varphi(x)$ is not convex. A sequence of lower-bounding piecewise-linear approximations of $\varphi(x)$ is built, which is tight for any given discrete choice of x , which guarantees that in a finite number of iterations the optimal solution can be found. Salmeron and Wood (2015) generalize this method for solving an interdiction problem of a power system whose lower-level problem is an MILP.

Lozano and Smith (2017b) introduce a backward-sampling approach for solving discrete interdiction problems. Sampling is used to create a subset of the follower’s solutions—optimizing over this subset gives the maximum perceived damage made by the leader and, hence, a valid lower bound. Similarly as in the method by Tang et al. (2016), the authors carefully extend the sampling set, while alternating between the calculations of the lower and upper bound, until the two values meet.

Finally, a combined column-and-row generation method, which relies on Benders decomposition, has been proposed by Zhao and Zeng (2013). The MILP model is dynamically extended by new variables that correspond to the follower’s response given a fixed leader’s decision x and the newly added constraints ensure the optimality condition for the follower’s response.

6.3. Critical Vertex/Edge Detection Problems in Graphs Seen Through the Lens of Bilevel Optimization.

Most of the existing literature dealing with detection of most vital arcs/vertices, with respect to some given graph-functionality measures, rely on extended MILP formulations; see, e.g., the recent survey by Lalou et al. (2018). Interesting applications include the maximization of the total number of pair-wise connected vertices while removing a limited number of arcs/vertices from the network (Arulselvan et al. 2009; Di Summa et al. 2012), the maximization of the number of connected components or the minimization of the size of the largest connected component (Shen and Smith 2012; Shen, Smith, and Goli 2012). Only recently, a connection between critical vertex/edge problems in graphs and

Stackelberg games has been exploited by Furini, Ljubić, Malaguti, et al. (2020) and Furini, Ljubić, Malaguti, et al. (2021), where the authors derive canonical formulations in the natural space of variables for the k -vertex cut and the capacitated vertex separator problem, respectively. The authors propose efficient B&C methods that beat the state-of-the-art thanks to the bilevel-like problem interpretation.

Finally, we point out that an up-to-date survey on network interdiction models and algorithms can be found in Smith and Song (2020). The survey also includes other aspects not covered in our survey such as interdiction under uncertainty, multilevel interdiction also known as defender-attacker-defender games (Baggio et al. 2021), as well as interesting problem extensions including situations in which both players act simultaneously, or problems with information asymmetry or information incompleteness (for either the leader or the follower).

7. POSSIBLE DIRECTIONS FOR FUTURE RESEARCH

The variety of aspects discussed in this survey show the required broadness of techniques that have to be exploited to solve bilevel optimization problems effectively. Despite the large amount of research carried out in the recent years, there are still very many aspects that need further investigation. In this section, we sketch a few of the many possible directions for future research in the field of computational bilevel optimization and begin with those aspects that are rather close to what is discussed in this paper.

- (1) The incorporation of integer variables in models is known to make the problem harder to solve. However, it is often easier to design provably correct algorithms for solving bilevel problems if all linking variables are integer. If this assumption does not hold, we have discussed in Section 5.1 that optimal solutions may not be attainable. This is the reason why more methods exist for ILP-ILP bilevel problems compared to what is published for the mixed-integer, i.e., the MILP-MILP, case. In this setting, solution methods need to deal with ε -optimality of solutions. This might be one reason why the performance of these methods is usually not comparable with the performance of methods that rely on the assumption of integer linking variables.
- (2) In this survey, we mainly discussed branch-and-bound as well as branch-and-cut methods for solving bilevel problems. We also mentioned a few primal heuristics. If one, however, compares the richness of cutting planes used in the field of single-level mixed-integer optimization with the number of known valid inequalities for bilevel optimization, it is obvious that many branch-and-cut algorithms would benefit from a larger set of bilevel-specific cutting planes. Moreover, the entire field of presolve techniques is almost completely unexplored in bilevel optimization, whereas the performance of state-of-the-art MILP solvers heavily relies on them.
- (3) If one compares the number of approaches for specific bilevel problems such as pricing problems as well as Stackelberg or interdiction games with the number of general-purpose approaches for bilevel LPs or bilevel MI(N)LPs, it becomes obvious that there still is a lot to do with respect to developing general-purpose algorithms for larger classes of bilevel problems. Of course, both previously mentioned aspects will also play a key role in developing further general-purpose methods.
- (4) In addition to the mathematical aspects mentioned so far, computational bilevel optimization still suffers from the absence of a broad variety of well-curated instance libraries that can be used to test and tune specific implementations of newly developed algorithms. Although some instance

sets are already publicly available (Paulavičius and Adjiman 2019; Ralphs 2020; Sinnl 2020; Zhou et al. 2020), the community of computational bilevel optimization would greatly benefit from more, and in particular more diverse, instance sets.

- (5) In addition, the development of novel algorithmic techniques would also very much benefit from more mature open-source realizations of “classical” methods in the field. Today, new ideas, e.g., for a novel valid inequality or a new presolve technique can usually only be tested if a lot of other techniques have been implemented on top of a basic branch-and-bound scheme. Obviously, availability of such open-source codes (of which MibS, see Ralphs (2018), is a notable example) would push the field significantly.

There are also many sub-areas of bilevel optimization that need to be developed further—especially when it comes to algorithmic and computational aspects. Let us exemplarily discuss two of them.

- (6) Most of the methods discussed in this survey tackle optimistic bilevel optimization problems. Although some important theoretical advances have been made in the field of pessimistic problems, the algorithmic treatment of these models is still in its infancy.
- (7) Another field worth to be mentioned is bilevel optimization under uncertainty—let it be stochastic or robust optimization problems embedded in a bilevel context. This problem class obviously is of tremendous importance for practice but, on the other hand, is also very hard to solve. The main reason is that the incorporation of uncertainty usually introduces another level in the problem, which then directly leads to tri- or general multilevel models that we will also comment on below again.

To sum up, there are many important and insufficiently explored topics in the field of bilevel optimization that lead to open research questions and, thus, to possible topics of future work. The focus of this survey is on mixed-integer programming techniques for solving challenging bilevel optimization problems. In this context, many interesting topics and questions arise that are at the interface of bilevel optimization and combinatorial optimization problems, problems from graph theory, algorithmic design, complexity theory, operations research, and applications. We are convinced that these connections can help us to derive tighter models, faster exact or approximation algorithms, or new structural properties. We sketch two exemplary problems at the interface of bilevel optimization as well as combinatorial optimization or graph theory:

- (8) The problem of generating a maximally violated valid inequality, i.e., the separation problem in a branch-and-cut context, can often be interpreted as a bilevel problem; see Lodi et al. (2014). In some cases, a compact single-level reformulation is not possible, and hence, any advancement in solving bilevel programs may have a significant impact on improving the performance of branch-and-cut based methods for difficult combinatorial optimization problems.
- (9) In graph theory, the families of critical vertex/edge detection problems, minimum d -blockers, or d -transversals in graphs can be formulated as bilevel (interdiction-like) optimization problems; see, e.g., Costa et al. (2011). This allows to look at some of the classical problems from graph theory from a different and fresh perspective and to possibly derive new mixed-integer formulations, which “live” in the canonical space of variables.

Moreover, many applications need to go beyond bilevel modeling and require tri- or even general multilevel models. This is, e.g., the case for interdiction problems with

fortification (Lozano and Smith 2017b), stochastic interdiction problems (Cormican et al. 1998), or for problems from energy market design (Grimm, Martin, et al. 2016). In this context, rather small scale instances are usually solved by exploiting hand-crafted and highly problem-specific solution methods. Thus, applied bilevel optimization would very much benefit from algorithmic enhancements for general tri- or multilevel problems.

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