# Bilevel mixed-integer linear programs and the zero forcing set*

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**Abstract.** We study a class of bilevel binary linear programs with lower-level variables in the upper-level constraints. Under certain assumptions, we prove that the problem can be reformulated as a single-level binary linear program, and propose a finitely terminating cut generation algorithm to solve it. We then relax the assumptions by means of a general row-and-column generation framework. As an illustrative application we consider the minimum zero forcing set problem, a variant of the dominating set problem, and prove that it can be written as a binary linear bilevel program. Finally, we perform some numerical experiments to showcase the practical applicability of our methods.

## 1 Introduction

A Bilevel Mixed-Integer Linear Program (BMILP) is a generalization of a standard Mixed-Integer Linear Program (MILP) which models a hierarchical decision process. The general formulation of a BMILP is:

$$(*)\left\{\begin{array}{lr} \min\limits_{x} \alpha^1 x + \alpha^2 y & \\ \quad Ax \geq b & (1) \\ \quad Gx + Hy \geq c & (2) \\ \quad x \in \mathcal{X} & (3) \\ \quad \left.\begin{array}{l} y \in \arg\min\limits_{y} \ \beta(x) y \\ \qquad\qquad y \in \Omega(x) \\ \qquad\qquad y \in \mathcal{Y} \end{array}\right\} & (4) \end{array}\right.$$

where $\alpha^1 \in \mathbb{Q}^n$, $\alpha^2 \in \mathbb{Q}^q$, $A \in \mathbb{Q}^{m\times n}$, $b \in \mathbb{Q}^m$, $G \in \mathbb{Q}^{p\times n}$, $H \in \mathbb{Q}^{p\times q}$, $c \in \mathbb{Q}^p$, $\beta(x) \in \mathbb{Q}^q$ is a linear function of $x$, $\Omega(x)$ is a polyhedron for each $x$, $\mathcal{X} = \mathbb{N}^{n_1} \times \mathbb{R}_+^{n_2}$, and $\mathcal{Y} = \mathbb{N}^{q_1} \times \mathbb{R}_+^{q_2}$. The variables of the problem are divided into two classes, the upper-level variables $x$ and the lower-level variables $y$. Similarly, the functions $(x, y) \mapsto \alpha^1 x + \alpha^2 y$ and $(x, y) \mapsto \beta(x)y$, are the upper-level and lower-level objective functions, respectively.

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The BMILP is a non-convex mixed-integer program. To the best of our knowledge no existing approach is able to solve ($*$) in full generality. However, as the interest in this problem has grown over the past years, several methods have been developed to solve some sub-classes of ($*$). One of the best studied cases is where the lower-level variables are continuous, i.e., $\mathcal{Y} = \mathbb{R}^q_+$ (see [3]). Under this condition, the lower-level problem (4) is convex and regular, and it can be replaced by its Karush-Kuhn-Tucker (KKT) conditions, yielding a single level reformulation of the problem. Several methods exist to solve this variant [2, 8].

Another well studied case is when $H = 0$, and $\beta(x) = \beta$, see [6, 9, 14]. In this case, at each iteration, the decision on the upper-level and the lower-level variables is taken separately. In particular, (i) the values of the upper-level variables subject to the restrictions of a set of upper-level constraints are found; (ii) the lower-level variables values are found by solving a MILP obtained by fixing the upper-level variable values previously found. The process iterates by updating the value of the upper-level variables.

A classic separation approach is applied to a relaxation of the problem in [6]. In [9], a basic implicit enumeration scheme is developed in order to find good feasible solutions within relatively few iterations. In [14], a scheme based on a reformulation and decomposition strategy is presented. The decomposition algorithm is based on the row-and-column generation method. The number of iterations needed for the convergence of this algorithm is shown to be finite.

The case where both sets $\mathcal{X}$ and $\mathcal{Y}$ are binary and $\beta(x)$ is a constant is considered in [13]. The problem is reduced to a multilevel linear program using a penalty function method. Solving the multilevel LP does not appear to offer a practically viable solution method. In [5, 10], the lower-level polyhedron $\Omega(x)$ does not depend on $x$, and the problem is solved using row generation.

In this paper we propose, to the best of our knowledge, the first practical method to solve the following BMILP variant: the upper-level variables $x$ are binary, $G$ and $H$ are one-row matrices, and $\beta(x) = \beta = H^\top$. Our motivation for studying this particular type of BMILP comes from a problem arising in the placement of electrical measurement devices on smart grids (see [12] and http://www.so-grid.com/), though our results apply to (and are therefore presented in terms of) general abstract BMILP formulations. Our contribution consists in treating the new case where lower-level variables appear in the upper-level constraints. We first prove that, under certain assumptions, it is possible to reformulate the BMILP into a single-level Binary Linear Program (BLP). This BLP, however, cannot be solved directly since the explicit polyhedral description of its constraints is not known. We therefore propose a finitely terminating cut generation algorithm. When the aforementioned assumptions do not hold, we propose a row-and-column generation framework. We also consider an application of our techniques to the minimum zero forcing set problem, introduced in [1], which consists in finding the minimum set of nodes in a graph that covers all the nodes given a specific propagation rule. We prove that this problem can be written as a BMILP problem and solved efficiently with our method.

The rest of the paper is organized as follows: in Section 2 and 3 we describe the single-level reformulation based on two specific assumptions, and propose a cut generation algorithm to solve the bilevel problem. In Section 4 we present a general framework for the case where the assumptions fail to hold. Finally, we prove that the minimum zero forcing set problem can be modeled as a binary bilevel program, and propose and test a practically viable solution algorithm in Section 5. All the proofs are reported in the appendix.

## 2 Bilevel Binary Linear Program

The standard Bilevel Binary Linear Program (BBLP) formulation is given by the following equivalent models:

$$\begin{cases} \min\limits_x \alpha x \\ \quad Ax \geq b \\ \quad x \in \{0,1\}^n \\ \quad \beta y \geq c - Gx \\ \quad \begin{cases} y \in \arg\min\limits_y \ \beta y \\ \qquad y \in \Omega(x) \\ \qquad y \in \mathcal{Y}. \end{cases} \end{cases} \equiv \begin{cases} \min\limits_x \alpha x \\ \quad Ax \geq b \\ \quad x \in \{0,1\}^n \\ \quad f(x) \geq c - \gamma x \\ \\ \quad f(x) = \begin{cases} \min\limits_y \ \beta y \\ \qquad y \in \Omega(x) \\ \qquad y \in \mathcal{Y} \end{cases} \end{cases}$$

where $\alpha \in \mathbb{Q}^n$, $A \in \mathbb{Q}^{m \times n}$, $b \in \mathbb{Q}^m$, $G \in \mathbb{Q}^{1 \times n}$, $c \in \mathbb{Q}$, $\beta \in \mathbb{Q}^q$, $\Omega(x)$ is a polyhedron for each $x$, $\gamma = G^\top$, and $\mathcal{Y} = \mathbb{N}^{q_1} \times \mathbb{R}_+^{q_2}$. The $x$ variables are the upper-level variables and the $y$ variables are the lower-level variables.

In order to formulate the BBLP as a single level program, we use the well-known lemma, which states that every subset of hypercube vertices has a linear description.

**Lemma 1.** *For any* $X \subset \{0,1\}^n$, $\mathsf{conv}(X) \cap \{0,1\}^n = X$.

Let $\mathcal{F} = \{x \in \{0,1\}^n \mid Ax \geq b \ \wedge f(x) \geq c - \gamma x\}$ be a linear description of the feasible set of the BBLP. By Lemma 1, the BBLP can be rewritten as the following Binary Linear Program (BLP): $\min\limits_x \{\alpha x \mid x \in \mathsf{conv}(\mathcal{F}) \cap \{0,1\}^n\}$.

Notice that, in general, a feasible upper-level variable $x$ for the continuous relaxation of the above BLP will not be feasible for the continuous relaxation of the corresponding BBLP. More precisely, in general the continuous relaxation of the BBLP is not convex, but the continuous relaxation of its linear reformulation (i.e., BLP) is obviously convex, since it is linear. However, if a polyhedral description of $\mathsf{conv}(\mathcal{F})$ is known, the linear reformulation of the BBLP allows us to solve the later using well known MILP solution methods.

In practice, it is difficult to compute a polyhedral description of $\mathsf{conv}(\mathcal{F})$. We therefore look for a polyhedron $\mathcal{P}$ such that $\mathcal{P} \cap \mathbb{Z}^n = \mathcal{F}$, i.e., a polyhedron

$\mathcal{P}$ containing $\mathsf{conv}(\mathcal{F})$, but no other binary point than those in $\mathsf{conv}(\mathcal{F})$. The BBLP can thus be formulated as: $\min_x \{\alpha x \mid x \in \mathcal{P} \cap \{0,1\}^n\}$.

First, we consider the *Restricted*-BBLP, i.e., the BBLP problem under the following hypotheses:

**Hypothesis 1** *For all $x, x' \in \{0,1\}^n$ such that $Ax \geq b$ and $Ax' \geq b$, if $x \leq x'$ then $\Omega(x) \supseteq \Omega(x')$. In other words, $f$ is a non-decreasing function over the set of $x$ such that $Ax \geq b$.*

**Hypothesis 2** *For all $i \in \{1, \ldots, n\}$, $\gamma_i \geq 0$.*

For any $S \subseteq \{0,1\}^n$, and a preorder $\preceq$ on $S$, we say that a point $s \in S$ is a $\preceq$-maximal point if no point $t \in S \setminus \{s\}$ is greater than $s$. Let us denote by $M(S)$ the set of $\leq$-maximal points in $S$, i.e., $M(S) = \{s \in S \mid \forall t \in S \ (t \geq s \rightarrow t = s)\}$. For any $v \in \{0,1\}^n$, let $\zeta(v) = \{i \leq n \mid v_i = 0\}$ be the complement of the support of $v$, where we recall that the support of a vector is the set of indices of its non-zero elements. Let $\bar{\mathcal{F}} = \{x \in \{0,1\}^n \mid Ax \geq b \wedge f(x) < c - \gamma x\}$ be the subset of $\{0,1\}^n$ which is feasible w.r.t. the "easy" constraints of the upper level, but infeasible w.r.t. the "hard" constraints (i.e., those involving the lower level). If $\bar{\mathcal{F}} = \varnothing$, the lower level problem can simply be removed. Therefore, assume in the following that $\bar{\mathcal{F}} \neq \varnothing$. We prove in the next section that a polyhedral description of $\mathsf{conv}(\mathcal{F})$ is obtained by adding valid inequalities generated using points in $M(\bar{\mathcal{F}})$.

# 3 A solution method for the Restricted-BBLP

## 3.1 A compact formulation of $\mathsf{conv}(\mathcal{F})$

In this section we describe the approach to build a "compact" polyhedron $\mathcal{P}$ such that $\mathcal{P} \cap \mathbb{Z}^n = \mathcal{F}$. We present a valid inequality for $\mathcal{F}$.

**Proposition 1.** *For all $\bar{x} \in \bar{\mathcal{F}}$, $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ is a valid inequality for $\mathcal{F}$.*

Let $\mathcal{P} = \{x \in [0,1]^n \mid Ax \geq b \wedge \forall \bar{x} \in M(\bar{\mathcal{F}}) \sum_{i \in \zeta(\bar{x})} x_i \geq 1\}$ and $\mathcal{P}_I = \mathcal{P} \cap \mathbb{Z}^n$. By Proposition 1, we have that $\mathcal{F} \subseteq \mathcal{P}_I$. In the following, we prove that $\mathcal{P}_I = \mathcal{F}$ and for all $\bar{x} \in M(\bar{\mathcal{F}})$, constraint $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ is a facet of $\mathcal{P}$.

**Proposition 2.** *The following statements hold: (i) $\mathcal{P}_I = \mathcal{F}$; (ii) for each $\bar{x} \in M(\bar{\mathcal{F}})$, $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ is a facet of $\mathcal{P}$.*

### 3.2 A cut generation algorithm

Now that we have a compact description polyhedron $\mathcal{P}$ such that $\mathcal{P} \cap \mathbb{Z}^n = \mathcal{F}$, we can build a constraint generation algorithm to solve $P$ under Hypotheses 1 and 2. We assume, without loss of generality, that $\Omega(x)$ is nonempty for at least some $x \in \{0,1\}^n$ such that $Ax \geq b$. The opposite would yield an infeasible lower-level problem, implying $f(x) = +\infty > c - \gamma x$ for any $x$. In other words, $P$ would reduce to a single-level MILP.

Algorithm 1 describes our cut generation algorithm for the *Restricted*-BBLP. The main idea is the following: assume that, at step $k$, we have a set $\mathcal{P}^k$ such that $\mathsf{conv}(\mathcal{F}) \subseteq \mathcal{P}^k$ and let $x^k$ be an optimal solution of the relaxed problem $P^k$: $\min_x \{\alpha x \mid x \in \mathcal{P}^k \cup \{0,1\}^n\}$. Then $x^k$ induces a lower bound for the *Restricted*-BBLP. Therefore, if $x^k \notin \mathcal{F}$, we have that $x^k \in \bar{\mathcal{F}}$. Since Hypothesis 1 is satisfied, we can find an element $\bar{x}^k \in M(\bar{\mathcal{F}})$ as explained in the next section. Therefore, at each iteration of Algorithm 1, either we find an optimal solution, or we add a facet of $\mathcal{P}$. Because rational polyhedra consist of a finite number of facets, Algorithm 1 will converge in finite number of iterations.

**Algorithm 1** Cut generation algorithm to solve the *Restricted*-BBLP

```
P^0 := {x ∈ [0,1]^n, | Ax ≥ b}
k := 0
x* := ∞
Condition := False
while Condition == False do
    Solve P^k and let x^k be an optimal solution
    x* ← x^k
    if f(x*) ≥ c − γx* then
        Condition ← True
    else
        Find x ≥ x* such that x ∈ M(F̄) (solve FM, see Section 3.3)
        x* ← x
        P^{k+1} := P^k ∩ {x | Σ_{i∈ζ(x*)} x_i ≥ 1}
        k ← k + 1
return x*
```

### 3.3 Finding maximal elements of $\bar{\mathcal{F}}$

We explain how, for an infeasible solution $\bar{x} \in \bar{\mathcal{F}}$, we can compute a maximal infeasible solution $x' \geq \bar{x}$, i.e., $x' \in M(\bar{\mathcal{F}})$. Consider, for a small enough $\varepsilon > 0$, the following single-level MILP:

$$\mathsf{FM} = \begin{cases} \max\limits_{x,y} \sum\limits_{i\in\zeta(\bar{x})} x_i \\ \qquad \beta\, y + \gamma\, x \leq c - \varepsilon \\ \qquad Ax \geq b \\ \qquad y \in \Omega(x) \\ \qquad x \geq \bar{x} \\ \qquad x \in \{0,1\}^n \\ \qquad y \in \mathcal{Y}. \end{cases}$$

Let $x \in \mathcal{F}$. Notice that, as $x \in \{0,1\}^n$ belongs to a finite set, there exists a small enough $\varepsilon > 0$ such that $x$ satisfies $Ax \geq b$ but not $\beta\, y + \gamma\, x \leq c - \varepsilon$, for any $y$. Now, we claim that the optimal solution $x^*$ of $\mathsf{FM}$, belongs to $M(\bar{\mathcal{F}})$. Indeed, since there exists $y \in \Omega(x^*)$ such that $\beta\, y + \gamma\, x^* < c$, we have that $f(x^*) < c - \gamma\, x^*$, i.e., $x^* \in \bar{\mathcal{F}}$. Furthermore, $x^* \geq \bar{x}$ hence $x^*$ dominates $\bar{x}$. If $x^* \notin M(\bar{\mathcal{F}})$, there must exist $x' \in \bar{\mathcal{F}}$ such that $\sum\limits_{i\in\zeta(\bar{x})} x'_i > \sum\limits_{i\in\zeta(\bar{x})} x^*_i$ which implies, by the optimality of $x^*$, that $\beta\, y + \gamma\, x' > c - \varepsilon$ for all $y$. Therefore, by the definition of $\varepsilon$, we have $x' \in \mathcal{F}$ which contradicts the initial assumption.
Notice that if $\varepsilon$ is not small enough, then the optimal solution $x^*$ of $\mathsf{FM}$ will dominate $\bar{x}$ but may not be maximal.

## 4 A solution method for the BBLP

In this section we explain how and to what extent it is possible to generalize the previous approach when Hypotheses 1 and 2 do not hold, and we propose a row-and-column generation algorithm.

### 4.1 Generalized domination in $\bar{\mathcal{F}}$

Let $B \in \mathbb{Q}^{r\times q}$, $C \in \mathbb{Q}^{r\times n}$, and $d \in \mathbb{Q}^r$ such that for all $x \in \{0,1\}^n$

$$\Omega(x) = \{y \in \mathbb{R}^q_+ \mid By \geq d + Cx\}.$$

Consider now $\bar{x} \in \bar{\mathcal{F}}$. In the following, we first prove that binary vectors dominated by $\bar{x}$ with respect to $C$ and $\gamma$ are infeasible. We also develop some nonlinear inequalities to separate these infeasible points from the feasible region $\mathcal{F}$. We then present a linear reformulation of these inequalities.

**Lemma 2.** *Let $\bar{x} \in \bar{\mathcal{F}}$. For all $x \in \{0,1\}^n$ such that $Ax \geq b$, $Cx \leq C\bar{x}$, and $\gamma x \leq \gamma\bar{x}$, we have that $x \notin \mathcal{F}$.*

Let $\mathcal{C}(\bar{x}) = \{x \in \mathbb{R}^n \mid \exists z \in \mathbb{R}^n\ (x = \bar{x} + z \wedge Cz \leq 0 \wedge \gamma z \leq 0)\}$. It is easy to see that $Cx \leq C\bar{x}$ and $\gamma x \leq \gamma\bar{x}$ if and only if $x \in \mathcal{C}(\bar{x})$. Let $\bar{x} \in \bar{\mathcal{F}}$ and $\Delta_{\bar{x}} : \{0,1\}^n \mapsto \mathbb{R}_+$ be the function defined by $\min\limits_{x'}\{\|x - x'\|_1 \mid x' \in \mathcal{C}(\bar{x})\}$.

**Lemma 3.** *Let $\bar{x} \in \bar{\mathcal{F}}$. $\Delta_{\bar{x}}$ defines a semimetric to the set $\mathcal{C}(\bar{x})$, i.e., for all $x \in \{0,1\}^n$, $\Delta_{\bar{x}}(x) \geq 0$ and $\Delta_{\bar{x}}(x) = 0$ if and only if $x \in \mathcal{C}(\bar{x})$.*

The optimization problem associated to $\Delta_{\bar{x}}(x)$ can be rewritten as follows:

$$\Delta_{\bar{x}}(x) = \begin{cases} \min\limits_{z,e,f} \ \sum\limits_{i=1}^{n} e_i + \sum\limits_{i=1}^{n} f_i \\ \qquad x = \bar{x} + z + e - f \\ \qquad Cz \leq 0 \\ \qquad \gamma z \leq 0 \\ \qquad e, f \in \mathbb{R}^n_+, \ z \in \mathbb{R}^n. \end{cases}$$

### 4.2 Valid nonlinear cuts

**Proposition 3.** *If $\bar{x} \in \bar{\mathcal{F}}$ then there exists $\delta_{\bar{x}} > 0$ such that inequality $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is valid for $\mathcal{F}$.*

We now show how to compute $\delta_{\bar{x}}$. Let $\bar{x} \in \bar{\mathcal{F}}$, $\varepsilon > 0$, and consider the following equivalent programs:

$$D_{\bar{x}}(\varepsilon) = \begin{cases} \min\limits_{x} \ \Delta_{\bar{x}}(x) \\ \quad \Delta_{\bar{x}}(x) \geq \varepsilon \\ \quad x \in \{0,1\}^n \end{cases} \equiv \begin{cases} \min\limits_{x,z,e,f} \ \sum\limits_{i=1}^{n} e_i + \sum\limits_{i=1}^{n} f_i \\ \qquad x - z - e + f = \bar{x} \\ \qquad Ax \geq b \\ \qquad Cz \leq 0 \\ \qquad \gamma z \leq 0 \\ \qquad \sum\limits_{i=1}^{n} e_i + \sum\limits_{i=1}^{n} f_i \geq \varepsilon \\ \qquad x \in \{0,1\}^n, \ e, f \in \mathbb{R}^n_+, \ z \in \mathbb{R}^n. \end{cases}$$

It is easy to see that taking $\varepsilon \leq \delta_{\bar{x}}$ will give an optimal solution $(x^*, z^*, e^*, f^*)$ of $D_{\bar{x}}(\varepsilon)$ such that $\sum\limits_{i=1}^{n} e^*_i + \sum\limits_{i=1}^{n} f^*_i = \delta_{\bar{x}}$. Therefore, if for some $\varepsilon$ we have $D_{\bar{x}}(\varepsilon) \leq \varepsilon$, then we can decrease the value of $\varepsilon$ and repeat the process until $D_{\bar{x}}(\varepsilon) > \varepsilon$, in which case $D_{\bar{x}}(\varepsilon) = \delta_{\bar{x}}$ holds.

### 4.3 Linearizing the cuts

Our inequalities are nonlinear since they are expressed as minimization problems. However, since these problems are LPs, we can replace them by their duals.

**Proposition 4.** *Let $\bar{x} \in \bar{\mathcal{F}}$. The constraint $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is equivalent to the system of inequalities:*

$$\begin{cases} \left. \begin{array}{l} (x - \bar{x})(C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}}) \geq \delta_{\bar{x}} \\ \\ -1 \leq C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}} \leq 1 \end{array} \right\} \mathcal{V}(\bar{x}) \\ \\ \sigma_{\bar{x}} \in \mathbb{R}^r_+, \ \vartheta_{\bar{x}} \in \mathbb{R}_+. \end{cases}$$

Notice that, if $x$ is not fixed, the constraint $(x-\bar{x})(C^\top\sigma_{\bar{x}}+\gamma\vartheta_{\bar{x}})\geq\delta_{\bar{x}}$ is not linear. Nevertheless, $x$ is a binary variable, and we can reasonably assume that $\sigma_{\bar{x}}$ and $\vartheta_{\bar{x}}$ are bounded, so we can reformulate the products $x_i\sigma_{\bar{x}j},\ x_i\vartheta_{\bar{x}}$ exactly by means of the Fortet reformulation [4].

### 4.4 Row-and-column generation algorithm for BBLP

We can now solve the BBLP in the general case using the same iterative framework as in Section 3. Assume that, at step $k$, we have a relaxation $\mathcal{Q}^k$ of $\mathsf{conv}(\mathcal{F})$ obtained by adding new variables $\sigma,\vartheta$, and constraints $\mathcal{V}(\bar{x})$ to $\mathcal{F}$. Let $x^k$ be an optimal solution of the relaxed problem: $Q^k=\min\limits_{x,\sigma,\vartheta}\{\alpha x\mid(x,\sigma,\vartheta)\in\mathcal{Q}^k, x\in\{0,1\}^n\}$ which generalizes $P^k$ introduced in Section 3.2. Then $x^k$ induces a lower bound for the original bilevel problem $P$ independently of Hypotheses 1 and 2. Therefore, if $x^k\in\mathcal{F}$, i.e., $f(x^k)\geq c-\gamma x^k$, we know that $x^k$ is an optimal solution of $P$. Otherwise, by Proposition 4, we add a set of new variables $\sigma,\vartheta$ and a set of new valid inequalities $\mathcal{V}(\bar{x}^k)$ to $\mathcal{Q}^k$ cutting all the binary points in $\mathcal{C}(\bar{x}^k)$, where $\bar{x}^k$ is chosen from $x^k$ in a similar way as in Section 3.

### 4.5 Finding $\leq_{\mathcal{C}}$-maximal elements of $\bar{\mathcal{F}}$

Let $\leq_{\mathcal{C}}$ be the partial preorder relation on $\{0,1\}^n$ such that $x^1\geq_{\mathcal{C}}x^2$ if and only if $Cx^1\geq Cx^2$ and $\gamma x^1\geq\gamma x^2$. In order to determine $\leq_{\mathcal{C}}$-maximal elements of $\bar{\mathcal{F}}$, we proceed as in Section 3. From an infeasible element $\bar{x}\in\bar{\mathcal{F}}$ we find another element $x'\in\bar{\mathcal{F}}$ for which $\mathcal{C}(x')$ is largest (so as to cut the largest number of infeasible points); or, in other words, a $\mathcal{C}$-maximal element $x'\in\bar{\mathcal{F}}$ which dominates $\bar{x}$. For any set $X\subset\{0,1\}^n$, we define $M_{\mathcal{C}}(X)$ as the set of maximal elements in $X$ under $\leq_{\mathcal{C}}$.

Let us consider the following optimization problem :

$$FM_C=\begin{cases}\max\limits_{x,y,e,f}\ \sum\limits_{i=1}^{m}e_i+f\\ \qquad\beta\,y+\gamma\,x\leq c-\varepsilon\\ \qquad Cx-e=C\bar{x}\\ \qquad\gamma\,x-f=\gamma\,\bar{x}\\ \qquad Ax\geq b\\ \qquad y\in\Omega(x)\\ \qquad e\geq0,\ f\geq0\\ \qquad x\in\{0,1\}^n\\ \qquad y\in\mathcal{Y}\end{cases}$$

for $\varepsilon>0$ small enough.

As in the previous section there exists a small enough $\varepsilon>0$ such that if $x$ satisfies $Ax\geq b$, but is infeasible in $\mathsf{FM_C}$, then $x\in\mathcal{F}$. We claim that the optimal solution $x^*$ of $\mathsf{FM_C}$ belongs to $M_C(\bar{\mathcal{F}})$. Notice first that by the second and third constraint of $\mathsf{FM_C}$, we have that $x^*\geq_C\bar{x}$. Furthermore, since there exists $y\in\Omega(x^*)$ such that $\beta\,y+\gamma\,x^*<c$, we have that $f(x^*)<c-\gamma\,x^*$,

i.e., $x^* \in \bar{\mathcal{F}}$. If $x^* \notin M_C(\bar{\mathcal{F}})$, there must exist $x' \in \bar{\mathcal{F}}$ and $(e', f')$ such that $\sum_{i=1}^{m} e'_i + f' > \sum_{i=1}^{m} e^*_i + f^*$, which implies by the optimality of $x^*$ that $\beta\, y + \gamma\, x' > c - \varepsilon$ for all $y$. Hence by definition of epsilon, we have that $x' \in \mathcal{F}$, which contradicts the initial assumption.

## 5 The minimum zero forcing set problem

We prove in this section that this problem can be modeled as a BBLP satisfying Hypotheses 1 and 2. The method proposed in this paper is also the first method solving the minimum zero forcing set problem.

### 5.1 The BBLP modeling

Let $G = (V, E)$ be a graph where $|V| = n$ and every vertex $v \in V$ has to be assigned an initial color, namely either black or white. We recall the definition of a zero forcing set of $G$, as it is given in [1]:

- *Color-change rule:* if $v \in V$ is a black vertex and all its neighbors (denoted by $\Gamma(v)$) are black besides one, say $u$, then change the color of $u$ to black.
- Given a coloring of $G$, the *derived coloring* is the result of applying the color-change rule until no more changes are possible.
- A *zero forcing set* for $G$ is a subset of black vertices $Z$ such that, if all the remaining vertices $V \setminus Z$ are white, the derived coloring of $G$ is all black.
- $Z(G)$ is the zero forcing set with minimum cardinality $|Z|$ over all zero forcing sets $Z \subseteq V$.

In [1], the authors prove that the size of a zero forcing set gives a bound on the minimum rank of the graph. We now prove that the problem of finding a minimum zero forcing set can be modeled as a BBLP. Let $Z \subseteq V$ be a nonempty set of vertices of $G$ colored in black, and let us define $S^0 = Z$. For each $t = 1, ..., n-1$, we define the set $S^t \subseteq V$ as the set of vertices $u \in V$ that are either in $S^{t-1}$ or whose color can be changed from white to black by an application of the color-change rule to a vertex $v \in S^{t-1}$. Notice that the derived coloring can be deduced from $S^{n-1}$.
Let $x \in \{0,1\}^n$ be the binary variable corresponding to the characteristic vector of $Z$ (i.e., $x_v = 1 \Leftrightarrow v \in Z$), and let $f(x)$ denote the size of the black vertices in $G$ in the derived coloring. The minimum zero forcing set problem can be modeled as the following program:

$$\begin{cases} \min\limits_{x} \sum\limits_{i=1}^{n} x_i \\ \qquad f(x) \geq |V| \\ \qquad x \in \{0,1\}^n. \end{cases}$$

We are given $x \in \{0,1\}^n$. In order to prove that $f(x)$ can be written as a binary program, we introduce the following function: $\theta^x : \{0,1\}^n \mapsto \{0,1\}^n$ such that each element of the vector $\theta^x(y)$ is given by:

$$\forall v \in V, \theta^x_v(y) = \max\left(x_v, y_v, \max_{u\in\Gamma(v)}\left(1 - |\Gamma(u)| + y_u + \sum_{\substack{v'\in\Gamma(u)\\ v'\neq v}} y_{v'}\right)\right).$$

For all $t = 1, ..., n-1$, let $y^t \in \{0,1\}^n$ denote the characteristic vector of set $S^t$. We have the following lemma.

**Lemma 4.** *For all $t = 1, ..., n-1$ we have $y^t = \theta^x(y^{t-1})$ where $y^0 = x$.*

Let $y = y^{n-1}$, then $y$ models the final colors of the vertexes in the derived coloring, i.e., 1 if black, 0 otherwise. From Lemma 4, we deduce that $y = \theta^x(y)$. Hence $y$ is a fixed point of $\theta^x$. Furthermore $y$ is a smallest fixed point of $\theta^x$ since if $\exists\ y' < y$ such that $y' = \theta^x(y')$ then the *color-change rule* cannot be applied further from the set $S'$ characterized by $y'$. Hence $|S'| < |S|$ which is a contradiction.
From these observations, we deduce that the value of $f(x)$ can be obtained by solving the following binary linear program:

$$f(x) = \begin{cases} \min\limits_{y} \sum\limits_{i=1}^{n} y_i \\ \quad y \geq x \\ \quad y_v \geq 1 - |\Gamma(u)| + y_u + \sum\limits_{\substack{v'\in\Gamma(u)\\ v'\neq v}} y_{v'},\ \forall v \in V, u \in \Gamma(v) \\ \quad y \in \{0,1\}^n. \end{cases}$$

Notice furthermore that Hypotheses 1 and 2 are satisfied.

### 5.2 Computational results

We tested the proposed algorithm using IBM ILOG CPLEX 12.6. The experiments were performed on an Intel i7 CPU at 2.70GHz with 16.0 GB RAM. The models were implemented in Julia using JuMP [7] . All the instances were solved to optimality and are feasible as $n$ is an upper bound on the feasible solution value and corresponds to coloring all the vertexes with black from the beginning.

In Table 1 we report the results of applying Algorithm 1 to the minimum zero forcing set problem on networks with topologies of standard IEEE $n$-bus systems [15], with $n \in \{5, 7, 14, 24, 30, 39, 57\}$. In Table 2, we report the results on randomly generated graphs with $n$ nodes and $1.4 \times n$ edges for $n = \{5 \times i, i = 1, \ldots, 10\}$ where 1.4 is the average rate of edges over nodes in standard IEEE bus systems. The instances can be forests and no node is isolated. For each tuple $(n, |E|)$, 10 instances are generated. In both cases, we report (the average over the 10 instances in Table 2):

- the CPU time expressed in seconds;
- the number |Iter|, of iterations of the algorithm;

- the optimal value $Val$;
- the effectiveness of the cuts when computed starting from the solution of problem FM (see Algorithm 1), i.e., maximal infeasible solution;
- the effectiveness of the cuts when computed starting from the solution of problem $P^k$ (see Algorithm 1), i.e., a potentially non-maximal infeasible solution.

The effectiveness reported in columns "FM" and "no_FM" is computed as the distance of the hyperplane represented by the cut and the infeasible point itself. In particular, we report the average distance over all the iterations for the proposed algorithm with or without solving FM, respectively. Note that for the "no_FM" case we report a best-case estimation because we do not consider that the number of iteration could also change, more precisely increase. Thus, the average effectiveness in this case could be worse than the one reported.

As expected the CPU time and the number of iterations needed to find the optimal solution increase as the size of the instance increases. Note also that the results presented in the two tables are comparable. In both case we can clearly see that solving FM provides always more effective cuts, thus showing the importance of generating the cut from a maximal infeasible solution.

In summary, the proposed algorithm appears to be a practical method to solve medium size instances of BBLP problem in a limited and reasonable amount of time.

| $n$ | $\|E\|$ | Time (s) | \|Iter\| | Val | FM | no_FM |
|---|---|---|---|---|---|---|
| 5 | 6 | 2.46 | 3 | 2 | 0.58 | 0.50 |
| 7 | 8 | 2.43 | 4 | 2 | 0.54 | 0.42 |
| 14 | 20 | 2.67 | 20 | 4 | 0.41 | 0.29 |
| 24 | 34 | 2.89 | 35 | 6 | 0.37 | 0.23 |
| 30 | 41 | 3.65 | 59 | 7 | 0.35 | 0.20 |
| 39 | 46 | 4.65 | 90 | 7 | 0.30 | 0.17 |
| 57 | 60 | 931.00 | 1150 | 9 | 0.23 | 0.14 |

Table 1: Results obtained for the minimum zero forcing set problem on networks with topologies of standard IEEE $n$-bus systems

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| $n$ | $\|E\|$ | Time (s) | \|Iter\| | Val | FM | no_FM |
|---|---|---|---|---|---|---|
| 5 | 7 | 2.66 | 4.20 | 2.20 | 0.59 | 0.52 |
| 10 | 14 | 2.72 | 8.20 | 3.20 | 0.48 | 0.34 |
| 15 | 21 | 2.64 | 19.80 | 4.10 | 0.42 | 0.29 |
| 20 | 28 | 2.86 | 42.90 | 5.20 | 0.38 | 0.25 |
| 25 | 35 | 3.22 | 69.60 | 5.80 | 0.35 | 0.22 |
| 30 | 42 | 6.00 | 126.00 | 6.90 | 0.33 | 0.20 |
| 35 | 49 | 11.90 | 204.60 | 7.10 | 0.30 | 0.18 |
| 40 | 56 | 20.00 | 286.90 | 9.10 | 0.30 | 0.17 |
| 45 | 62 | 85.60 | 484.30 | 8.80 | 0.26 | 0.17 |
| 50 | 70 | 563.30 | 1021.60 | 10.50 | 0.26 | 0.15 |

Table 2: Results obtained for the minimum zero forcing set problem on random graphs


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## A Proofs

In the following, we provide the missing proofs of all the results stated in the paper.

**Proposition 1.** *For all $\bar{x} \in \bar{\mathcal{F}}$, $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ is a valid inequality for $\mathcal{F}$.*

*Proof.* Assume there exists $x \in \mathcal{F}$ such that $\sum_{i \in \zeta(\bar{x})} x_i < 1$. Since $x \in \{0,1\}^n$ we have that $\sum_{i \in \zeta(\bar{x})} x_i = 0$, which implies that, for all $i \in \zeta(\bar{x})$, $x_i = 0$. Hence $x \leq \bar{x}$ and $f(x) \leq f(\bar{x}) < c - \gamma\bar{x}$ by Hypothesis 1. Therefore by Hypothesis 2, we conclude that $f(x) < c - \gamma x$, contradicting the assumption. □

**Proposition 2.** *The following statements hold: (i) $\mathcal{P}_I = \mathcal{F}$; (ii) For each $\bar{x} \in M(\bar{\mathcal{F}})$, $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ is a facet of $\mathcal{P}$.*

*Proof.* (i) Let $x \in \mathcal{P}_I$ and suppose, to get a contradiction, that $x \notin \mathcal{F}$. By definition, $x \in \bar{\mathcal{F}}$. Pick a $\bar{x} \in M(\bar{\mathcal{F}})$ such that $\bar{x} \geq x$. Since $x \in \mathcal{P}_I$ and $\bar{x} \in M(\bar{\mathcal{F}})$, we have, by definition of $\mathcal{P}_I$, that $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ $(*)$. However, since $\bar{x}, x$ are binary vectors and $\bar{x} \geq x$, it follows that $x_i = 0$ for all $i \leq n$ such that $\bar{x}_i = 0$. This means that $\sum_{i \in \zeta(\bar{x})} x_i = 0$, against $(*)$. Therefore $x \in \mathcal{F}$ and $\mathcal{P} \cap \mathbb{Z}^n = \mathcal{F}$ as claimed.
(ii) Let $\bar{x} \in M(\bar{\mathcal{F}})$. Let us now prove that $\sum_{i \in \zeta(\bar{x})} x_i \geq 1$ $(\dagger)$ is a facet of $\mathcal{P}$. Suppose, to get a contradiction, that removing $(\dagger)$ from the definition of $\mathcal{P}$ yields $\mathcal{P}$ again. Since $\bar{x} \in M(\bar{\mathcal{F}})$, $\bar{x} \in \bar{\mathcal{F}}$. Note that for any $x' \in \bar{\mathcal{F}}$ we have $\sum_{i \in \zeta(x')} x'_i = 0$ by definition of $\zeta$. Thus by Proposition 1 and by definition of $\mathcal{P}$, $x' \notin \mathcal{P}$ and in particular $\bar{x} \notin \mathcal{P}$. Then there must be some inequality in the definition of $\mathcal{P}$ which cuts off $\bar{x}$, and none of the inequalities in $Ax \geq b$ qualify since, by definition of $\bar{\mathcal{F}}$, $A\bar{x} \geq b$. Hence it must be one of the other inequalities, say $\sum_{i \in \zeta(x')} x_i \geq 1$ for some $x' \in M(\bar{\mathcal{F}})$ with $x' \neq \bar{x}$. This means that $\sum_{i \in \zeta(x')} \bar{x}_i = 0$ which implies that $\bar{x}_i = 0$ for all $i \leq n$ such that $x'_i = 0$. Together with $x' \neq \bar{x}$, it follows that $\bar{x} < x'$, which contradicts the maximality of $\bar{x}$ in $\bar{\mathcal{F}}$. □

**Lemma 2.** *Let $\bar{x} \in \bar{\mathcal{F}}$. For all $x \in \{0,1\}^n$ such that $Ax \geq b$, $Cx \leq C\bar{x}$, and $\gamma x \leq \gamma\bar{x}$, we have that $x \notin \mathcal{F}$.*

*Proof.* Let $\bar{y} \in \Omega(\bar{x})$ such that $f(\bar{x}) = \beta\bar{y} < c - \gamma\bar{x}$. Since $Cx \leq C\bar{x}$, we have that $B\bar{y} \geq d + Cx$. Hence $\bar{y} \in \Omega(x)$. Therefore $f(x) \leq f(\bar{x}) < c - \gamma\bar{x}$ $(*)$. However, since $\gamma x \leq \gamma\bar{x}$ and $\bar{x}$ is subtracted from $c$ in the RHS of $(*)$, we deduce that $f(x) < c - \gamma x$ and therefore $x \notin \mathcal{F}$. □

**Lemma 3.** *Let $\bar{x} \in \bar{\mathcal{F}}$. $\Delta_{\bar{x}}$ defines a semimetric to the set $\mathcal{C}(\bar{x})$, i.e., for all $x \in \{0,1\}^n$, $\Delta_{\bar{x}}(x) \geq 0$ and $\Delta_{\bar{x}}(x) = 0$ if and only if $x \in \mathcal{C}(\bar{x})$.*

*Proof.* The function $\Delta_{\bar{x}}$ is positive by definition. Assume that there exist $x \in \{0,1\}^n$ such that $\Delta_{\bar{x}}(x) = 0$ and let $x^*$ be the optimal solution of the optimization problem associated to $\Delta_{\bar{x}}(x)$. By definition, $x = x^*$, and then $x \in \mathcal{C}(\bar{x})$. Conversely, if $x \in \mathcal{C}(\bar{x})$ then we can set $x' = x$ which conclude the proof. □

**Proposition 3.** *If $\bar{x} \in \bar{\mathcal{F}}$ then there exists $\delta_{\bar{x}} > 0$ such that inequality $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is valid for $\mathcal{F}$.*

*Proof.* Let $\delta_{\bar{x}} = \min_{x \in \mathcal{F}} \Delta_{\bar{x}}(x)$. Since $\mathcal{F}$ is a finite set, $\delta_{\bar{x}}$ exists. Suppose, to get to a contradiction, that $\delta_{\bar{x}} = 0$. Then there must exist $x \in \mathcal{F}$ such that $\Delta_{\bar{x}}(x) = 0$, which implies that $x \in \mathcal{C}(\bar{x})$ by Lemma 3. Also, since $x \in \mathcal{F}$, we have in particular that $Ax \geq b$. However, Lemma 2 states that for each $\bar{x} \in \bar{\mathcal{F}}$ and $x \in \{0,1\}$ with $Ax \geq b$, if $x \in \mathcal{C}(\bar{x})$ then $x \notin \mathcal{F}$, which contradicts the assumption $x \in \mathcal{F}$; hence $\delta_{\bar{x}} > 0$. Furthermore, by definition of $\delta_{\bar{x}}$, we have that the inequality $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is valid for $\mathcal{F}$. □

**Proposition 4.** *Let $\bar{x} \in \bar{\mathcal{F}}$. The constraint $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is equivalent to the system of inequalities:*

$$\begin{cases} (x - \bar{x})(C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}}) \geq \delta_{\bar{x}} \\ -1 \leq C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}} \leq 1 \\ \sigma_{\bar{x}} \in \mathbb{R}^r_+, \ \vartheta_{\bar{x}} \in \mathbb{R}_+. \end{cases}$$

*Proof.* Let us recall the LP formulation of $\Delta_{\bar{x}}(x)$:

$$\Delta_{\bar{x}}(x) = \begin{cases} \min\limits_{z,e,f} \ \sum\limits_{i=1}^{n} e_i + \sum\limits_{i=1}^{n} f_i \\ \qquad x = \bar{x} + z + e - f \\ \qquad Cz \leq 0 \\ \qquad \gamma z \leq 0 \\ \qquad e, f \in \mathbb{R}^n_+, \ z \in \mathbb{R}^n \end{cases}$$

For all $x \in \{0,1\}^n$, we introduce its dual, $\Pi_{\bar{x}}(x)$:

$$\Pi_{\bar{x}}(x) = \begin{cases} \max\limits_{\sigma_{\bar{x}}, \vartheta_{\bar{x}}} \ (x - \bar{x})(C\sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}}) \\ \qquad -1 \leq C\sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}} \leq 1 \\ \qquad \sigma_{\bar{x}} \in \mathbb{R}^r_+, \ \vartheta_{\bar{x}} \in \mathbb{R}_+ \end{cases}$$

Since $\Delta_{\bar{x}}(x)$ has always a finite optimal solution, by the strong duality theorem of LP, we have that the optimal values of the primal and of the dual are equal. Therefore the constraint $\Delta_{\bar{x}}(x) \geq \delta_{\bar{x}}$ is equivalent to $\Pi_{\bar{x}}(x) \geq \delta_{\bar{x}}$. However, given the expression of the dual, we conclude that $\Pi_{\bar{x}}(x) \geq \delta_{\bar{x}}$ if and only if there exist $\sigma_{\bar{x}} \in \mathbb{R}^r_+, \ \vartheta_{\bar{x}} \in \mathbb{R}_+$ such that:

$$\mathcal{V}(\bar{x}) = \begin{cases} (x - \bar{x})(C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}}) \geq \delta_{\bar{x}} \\ -1 \leq C^\top \sigma_{\bar{x}} + \gamma \vartheta_{\bar{x}} \leq 1 \end{cases}$$

is verified, as claimed. □

**Lemma 4.** *For all* $t = 1, ..., n$ *we have:*

$$y^t = \theta^x(y^{t-1})$$

*where* $y^0 = x$.

*Proof.* Let $v \in V$. By definition, $\theta_v^x(y^{t-1}) = \max(x_v, y_v^{t-1}, Q)$ where $Q = \max_{u\in\Gamma(v)}(1 - |\Gamma(u)| + y_u^{t-1} + \sum_{\substack{v' \in \Gamma(u)\\ v' \neq v}} y_{v'}^{t-1})$. We have $Q \leq 1$, hence $\theta_v^x(y^{t-1}) \in \{0, 1\}$.

- If $x_v = 1$ or $y_v^{t-1} = 1$, then $v \in S^{t-1}$ and hence $v \in S^t$. Therefore $y_v^t = \theta_v^x(y^{t-1}) = 1$.
- Assume now that$x_v = y_v^{t-1} = 0$. We prove that $Q = 1$ if and only if the color of $v$ can be changed from white to black using a vertex $u \in \Gamma(v)$. Indeed, $Q = 1$ if and only if there exists a vertex $u \in \Gamma(v)$ such that $y_u^{t-1} = 1$ and $y_{v'}^{t-1} = 1$ for all $v' \in \Gamma(u)$ with $v' \neq v$. Such a case happens when $v$ has a neighbor $u$ colored in black with all its other neighbors $v' \in \Gamma(u) \setminus \{v\}$ colored in black. Then $v \in S^t$. Therefore the function $\theta^x$ models the *color-change rule* of $G$ when the initial vertices colored in black are modeled by $x$.

Therefore, $y^t = \theta^x(y^{t-1})$. □