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Cliques, holes and the vertex coloring polytope

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Abstract

Certain subgraphs of a given graph G restrict the minimum number $\chi(G)$ of colors that can be assigned to the vertices of G such that the endpoints of all edges receive distinct colors. Some of such subgraphs are related to the celebrated Strong Perfect Graph Theorem, as it implies that every graph G contains a clique of size $\chi(G)$, or an odd hole or an odd anti-hole as an induced subgraph. In this paper, we investigate the impact of induced maximal cliques, odd holes and odd anti-holes on the polytope associated with a new 0–1 integer programming formulation of the graph coloring problem. We show that they induce classes of facet defining inequalities.
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1. Introduction

Given a graph $G = (V, E)$, where V is its set of vertices and E its set of edges, and a positive integer k, a k*-coloring* of G (or, more generally, a *coloring* of G) is an assignment of colors from $\{1, \dots, k\}$ to the vertices of G so that each vertex receives at least one color and the endpoints of all edges are assigned different colors. The *graph coloring problem* is defined as the problem of finding the minimum number of colors $\chi(G)$, known as the *chromatic number* of G, such that G admits a $\chi(G)$-coloring. Observe that there exists a coloring of G with $\chi(G)$ colors in which each vertex is assigned exactly one color.

Describing optimal solutions of the graph coloring problem is one of the most challenging problems in combinatorial optimization. One possible approach is to formulate the problem as a 0–1 integer program. This approach has received a considerable attention in the last years, as the formulations depicted in Table 1 indicate. The notation adopted in the table is n for the number of vertices of G, m for its number of edges and $\overline{m}$ for the number of edges of the complement of G. For each formulation, it is presented the number of binary variables employed, the number of linear constraints, the dimension of the corresponding polytope and a reference in the literature.

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Table 1
0–1 integer programming formulations of the graph coloring problem from the literature

Formulation	Variables	Constraints	Dimension
Independent sets [7]	Exponential	$O(n)$	–
Color per vertex [3,4]	$O(n^2)$	$O(nm)$	$n^2 - \chi(G) - 1$
Acyclic orientations [5]	$O(n+m)$	Exponential	$2n + 4m$
Representatives	$O(n+\overline{m})$	$O(nm)$	$n + 2\overline{m}$

The first formulation mentioned in the table was exploited by Mehrotra and Trick in a branch-and-bound algorithm described in [7]. This formulation, called MIS (for *maximal independent sets*), uses a binary variable for each maximal independent set of the graph. Handling such an exponential number of variables constitutes an apparent drawback of the MIS formulation. For this reason, some authors have proposed more compact alternative formulations. For instance, Díaz and Zabala adopted a formulation that uses a variable to each possible color and vertex [3,4]. Alternatively, Figueiredo et al. formulated the graph coloring problem in terms of an optimization problem over the set of acyclic orientations of the graph [5]. Partial studies of the facial structure of the polytopes associated with these alternative formulations are presented, respectively, in [3] and [5].

In this paper, we propose a new 0–1 integer programming formulation which is simpler and more compact than other formulations in the literature. We also present a partial study of the structure of the polytope $P(G)$ associated with this formulation. We show that certain particular substructures of G induce classes of facet defining inequalities. One example of such substructures is a maximal clique of the graph. Since the size of any clique in the graph is a trivial lower bound of $\chi(G)$, it seems natural that maximal cliques induce constraints of $P(G)$ (this turns out to be indeed the case for the formulations studied in [3] and [5]). However, cliques are not sufficient to express all the intricate structural aspects related to graph coloring. This is demonstrated by the existence of triangle-free graphs with chromatic number arbitrarily larger than 2 [6].

The celebrated Strong Perfect Graph Theorem identifies two more substructures by stating that G contains a clique of size $\chi(G)$, or an odd hole or an odd anti-hole as an induced subgraph [1,2]. Not surprisingly, then, is that odd holes and anti-holes also have some influence in $P(G)$. We show some facet defining inequalities based on them.

The rest of the paper is organized as follows. The new 0–1 formulation is presented in Section 2. Section 3 is devoted to the description of some structural properties of $P(G)$, including facet defining inequalities based on maximal cliques and odd holes and anti-holes. Finally, we close the paper with some conclusions and further directions in Section 4.

2. Representative formulation

Throughout this paper, $G = (V, E)$ is a simple and connected graph. Let us denote $|V|$ by n, $|E|$ by m, by $\overline{G} = (V, \overline{E})$ the complementary graph of G and $|\overline{E}|$ by $\overline{m}$. For $v \in V$, $N(v)$ denotes the neighborhood of v in G, while in $\overline{G}$ the neighborhood of v is denoted $\overline{N}(v)$. Define $N[v] = N(v) \cup \{v\}$ and $\overline{N}[v] = \overline{N}(v) \cup \{v\}$. Let $S \subseteq V$. For the sake of simplicity of notation, $S + v$ and $S - v$ stand for $S \cup \{v\}$ and $S \backslash \{v\}$, respectively. The common anti-neighborhood of S is given by $\overline{N}(S) = \bigcap_{v \in S} \overline{N}(v)$. Write $E[S]$ for the set of edges of $G[S]$, which in turn is the subgraph of G induced by S. If S is such that $u, v \in S$ yields $uv \notin E$, then S is an *independent set* of G. We use the easy facts:

(1) If $u \in V$ satisfies $\overline{N}(u) = \emptyset$ (in which case it is called *universal*), then $\chi(G) = \chi(G - u) + 1$.
(2) If $u \in V$ and $S \subseteq \overline{N}(u)$ is a set of *isolated vertices* in $G[\overline{N}(u)]$, that is $E[\overline{N}(u)] = E[\overline{N}(u) \setminus S]$, then $\chi(G) = \chi(G - S)$.

to make the following assumption.

Assumption 1. G has no universal vertices and the anti-neighborhood of every vertex of G has no isolated vertices.

A coloring of G can be viewed as a family $S_1, \ldots, S_k$ of $k \geqslant \chi(G)$ independent sets of G, each independent set in the family associated with a color. Suppose that, for each color i, we choose a vertex to be the representative of the corresponding color class S_i. Then, each vertex can be in one of two states: either it represents its color or there exists another vertex that represents its color. To describe such a situation, define the binary variables x_{uv}, for all $u \in V$ and $v \in \overline{N}[u]$, with the following interpretation: $x_{uv} = 1$ if and only if u represents the color of v. A vector x^* that comprises all of these binary variables is an incidence vector of a $\chi(G)$-coloring of G if, and only if, it minimizes $\sum_{v \in V} x_{vv}$ over all binary vectors x such that

$$\sum_{u \in \overline{N}[v]} x_{uv} \geqslant 1, \tag{1}$$

for all $v \in V$ and, for all $u \in V$ and $vw \in E[\overline{N}(u)]$,

$$x_{uv} + x_{uw} \leqslant x_{uu}. \tag{2}$$

Constraints of type (1) indicate that each vertex $v \in V$ must be represented either by itself or by some vertex in its anti-neighborhood. Since the endpoints of every edge must be assigned distinct colors, constraints of type (2) assure that they have distinct representatives. Observe that if $u \in V$ and $v \in \overline{N}(u)$, then the inequality $x_{uv} \leqslant x_{uu}$ is a consequence of constraints (2) related to u, since it is assumed that there are no isolated vertices in $G[\overline{N}(u)]$.

The representative formulation described above is referred to as REP, for short. It can be seen as a variation of the MIS formulation that uses only $n + 2\overline{m}$ binary variables to represent the independent sets of the graph.

3. On the coloring polytope

Now, we turn our attention to the polytope $P(G) = \operatorname{conv}\{x \in \{0,1\}^{n+2\overline{m}} \mid x$ satisfies (1) and (2)$\}$. Given a pair of (not necessarily distinct) vertices $u, v \in V$, $uv \notin E$, the incidence vector of uv is x^{uv}, defined in the following way: for each $u' \in V$ and $v' \in \overline{N}[u']$, if $u' = u$ and $v' = v$, then $x^{uv}_{u'v'} = 1$; otherwise, $x^{uv}_{u'v'} = 0$. The following incidence vectors in $P(G)$ are useful in the proofs of this section:

- $X = \sum_{u \in V} x^{uu}$.
- $X^{\bar{u}} = X - x^{uu} + x^{ru}$, for $u \in V$ and a representative $r \in \overline{N}(u)$.
- $X^{uv} = X + x^{uv}$, for $u \in V$ and $v \in \overline{N}(u)$.

First, the dimension of $P(G)$ is established next.

Lemma 2. *$P(G)$ is full-dimensional, i.e.,* $\dim(P(G)) = n + 2\overline{m}$.

Proof. Let us consider the following $n + 2\overline{m} + 1$ distinct vectors in $P(G)$: X, $X^{\bar{u}}$ and X^{uv}, for all $u \in V$ and $v \in \overline{N}(u)$. To show that they are affinely independent, consider a_0, a_{uv} ($u \in V, v \in \overline{N}(u)$) and a_u ($u \in V$), all of them in $\mathbb{R}$, such that

$$A = a_0 + \sum_{u \in V} a_u + \sum_{u \in V,\ v \in \overline{N}(u)} a_{uv} = 0 \tag{3}$$

and

$$a_0 X + \sum_{u \in V} \left(a_u X^{\bar{u}} + \sum_{v \in \overline{N}(u)} a_{uv} X^{uv} \right) = 0. \tag{4}$$

The x_{ww} entries of each term in Eq. (4) give $A - a_w = 0$, for all $w \in V$. This fact, together with (3), results that $a_w = 0$. Now, considering the x_{wz} entries, for all $w \in V$, $z \in \overline{N}(w)$, we easily get $a_{wz} = 0$. Finally, Eq. (3) implies $a_0 = 0$. Therefore, we have $2\overline{m} + n + 1$ affinely independent vectors, as required. □

The facets described in the following theorem, along with those in Corollary 6, are sufficient to ensure that all variables of $P(G)$ belong to the interval [0, 1].

Theorem 3. *Bounding inequalities $x_{uu} \leqslant 1$ and $x_{uv} \geqslant 0$, for each $u \in V$ and $v \in \overline{N}(u)$, give facets of $P(G)$.*

Proof. To prove each case of the theorem, we exhibit $n + 2\overline{m}$ affinely independent vectors that satisfy the corresponding inequality at equality. Let $u \in V$ and $v \in \overline{N}(u)$. First, observe that $x_{uu} = 1$ holds for all vectors X and X^{wz} and $X^{\bar{w}}$, for all $w \in V$ and $z \in \overline{N}(w)$, except for $X^{\bar{u}}$. By the proof of Lemma 2, all of these $n + 2\overline{m}$ vectors are affinely independent. Further, for the inequality $x_{uv} \geqslant 0$, again it is satisfied at equality by all vectors X, X^{wz} and $X^{\bar{w}}$ but just X^{uv}, and this if we choose a representative $r \neq u$ for v in the definition of $X^{\bar{v}}$. Such a choice is possible since $\overline{N}(v)$ is not a singleton, by Assumption 1. □

In each of the following theorems, in order to prove that a face $F' = \{x \in P(G) \mid \lambda' x = \beta'\}$ defines a facet of $P(G)$, we show that if a facet $F = \{x \in P(G) \mid \lambda x = \beta\}$ of $P(G)$ contains F', then there exists $a \in \mathbb{R}$ such that $\lambda = a\lambda'$ and $\beta = a\beta'$ [8]. We start with constraints of type (1) of REP.

Theorem 4. *For each $v \in V$, the vertex inequality $\sum_{u \in \overline{N}[v]} x_{uv} \geqslant 1$ is a facet defining inequality of $P(G)$.*

Proof. Let F' be the face $\{x \in P(G) \mid \sum_{u \in \overline{N}[v]} x_{uv} = 1\}$ of $P(G)$. It follows from $F' \subseteq F$ that F contains X and $X - x^{zz} + x^{wz}$, for every $z \in V$ and $w \in \overline{N}(z)$. Consequently, $\lambda X = \lambda(X - x^{zz} + x^{wz}) = \beta$, leading to $\lambda(x^{wz} - x^{zz}) = \lambda_{wz} - \lambda_{zz} = 0$, and $\lambda_{zz} = \lambda_{wz}$. If we take $z \neq v$, then $X + x^{wz}$ also belongs to F, which means that $\lambda(X + x^{wz}) = \beta$. Thus, $\lambda x^{wz} = \lambda_{wz} = 0$. Therefore, $\lambda x = \lambda_{vv} \sum_{u \in \overline{N}[v]} x_{uv}$, which concludes the proof. $\square$

Next, we present two classes of facet defining inequalities related to substructures of G. First, given $H \subseteq V$, let us denote by α_H the maximum size of an independent set of $G[H]$.

Theorem 5. *Let $u \in V$ and $H \subseteq \overline{N}(u)$. The independent set inequality $\sum_{v \in H} x_{uv} \leqslant \alpha_H x_{uu}$ is valid for $P(G)$. Moreover, it is facet defining if the following properties hold*:

(P1) $G[H]$ *is* α_H-maximal, *which means that if $\overline{N}(u) \supset H' \supset H$, then $\alpha_{H'} > \alpha_H$; and*
(P2) *the graph formed by H and the safe edges of $G[H]$ is connected, where an edge vw in $G[H]$ is said to be* safe *if there exist two maximum independent sets S_v and S_w of $G[H]$ such that $S_v \backslash S_w = \{v\}$ and $S_w \backslash S_v = \{w\}$.*

Observe that property (P1) above and Assumption 1 imply that $|H| \geqslant 2$.

Proof. Consider $u \in V$, $H \subseteq \overline{N}(u)$ and an incidence vector x of a coloring of G. If $x_{uu} = 0$, then u cannot be the representative of any vertex. Otherwise, if $x_{uu} = 1$, then the vertices of H represented by u form an independent set, whose size is at most α_H. Then, the inequality is valid.

Now consider that properties (P1) and (P2) hold for H. Let $F' = \{x \in P(G) \mid \sum_{v \in H} x_{uv} - \alpha_H x_{uu} = 0\}$, $w \in V$, $z \in \overline{N}(w)$ and S be a maximum independent set of $G[H]$. Write $X^S = \sum_{v \in V} x^{vv} + \sum_{v \in S} x^{uv}$, and notice that $X^S \in F' \subseteq F$.

First, we show the zero entries of λ. The vectors X^S and $X^S + x^{wz}$, both in F, prove that $\lambda_{wz} = 0$ when $w \neq u$. They also prove the same result when $w = u$ and $z \notin H$, in which case we need $S + z$ to be an independent set of G because, otherwise, inequality (2) would be violated by z and any neighbor of it in S. Property (P1) ensures that such an S exists. In addition, to prove that $\lambda_{ww} = 0$ when $w \neq u$, we consider the points $X^S + x^{zw}$ and $X^S + x^{zw} - x^{ww}$. They belong to F if we choose $z \neq u$, which is possible because $|\overline{N}(w)| \geqslant 2$ by Assumption 1.

Let us examine the non-zero entries now. Initially, consider a safe edge vw of $G[H]$. Choose maximum independent sets S_v and S_w such that $S_v \backslash S_w = \{v\}$ and $S_w \backslash S_v = \{w\}$. It turns out that both X^{S_v} and X^{S_w} belong to F, meaning that $\lambda_{uv} = \lambda_{uw}$. By the connectivity condition established by property (P2), $\lambda_{uv} = \lambda_{uw}$ extends for every $v, w \in H$. Finally, still suppose that $w \in H$. To show the relationship between the entries of λ associated with uu and uw, consider the points $X^S + x^{wu}$ and $X^{wu} - x^{uu}$. Since both belong to F, we get $0 = \lambda(x^{uu} + \sum_{v \in S} x^{uv}) = \lambda_{uu} + \alpha_H \lambda_{uw}$. Thus, $\lambda_{uu} = -\alpha_H \lambda_{uw}$ and the sufficient condition of the theorem follows. $\square$

It is immediate to see that the properties of the latter theorem hold for maximal cliques. More precisely, we have

Corollary 6. *Let $u \in V$ and $K \subseteq \overline{N}(u)$ such that $G[K]$ is a maximal clique of $G[\overline{N}(u)]$. Then, the clique inequality $\sum_{v \in K} x_{uv} \leqslant x_{uu}$ is a facet defining inequality of $P(G)$.*

The previous corollary has two important consequences. First, clique inequalities and the facet defining inequalities of Theorem 3 imply that all variables of $P(G)$ belong to the interval $[0, 1]$. Hence, $x_{uu} \geqslant 0$ and $x_{uv} \leqslant 1$, for all $u \in V$ and $v \in \overline{N}(u)$, do not define facets of $P(G)$. Second, constraint of type (2) does not define a facet of $P(G)$ if vw is not a maximal clique of $\overline{N}(u)$. The argument here is that whenever (2) is satisfied at equality, so is the clique inequality for a maximal clique of $G[\overline{N}(u)]$ that contains vw.

Define an *odd hole* as an induced chordless cycle on an odd number of vertices, and an *odd anti-hole* as the complement of an odd hole. Theorem 5 is also concerned with these substructures.

Corollary 7. *If $u \in V$, $H \subset \overline{N}(u)$ induces an odd hole or anti-hole, and property* (P1) *of Theorem* 5 *holds, then the independent set inequality associated with u and H is a facet defining inequality of $P(G)$.*

Next, we establish the second class of facet defining inequalities associated with substructures of G. We say that a subgraph $G[H]$ of G is $\chi(G[H])$*-critical* if $\chi(G[H-v]) = \chi(G[H]) - 1$, for all $v \in H$.

Theorem 8. *If $H \subseteq V$, then*

$$\sum_{v \in H} x_{vv} + \sum_{v \in H} \sum_{u \in \overline{N}(v) \setminus H} x_{uv} \geqslant \chi\bigl(G[H]\bigr) \tag{5}$$

is a valid inequality for $P(G)$. In addition, the chromatic number inequality (5) *is facet defining if $G[H]$ is $\chi(G[H])$-critical and $\overline{G}[H]$ is connected.*

Notice that if $|H| = 1$, then we have the vertex inequality considered in Theorem 4. Thus, we assume in the proof that $|H| \geqslant 2$.

Proof. In any coloring of G, each color appearing in H adds 1 either to the first or to the second term of the left hand-side of inequality (5). Since at least $\chi(G[H])$ colors are necessary to color $G[H]$, this inequality is valid.

Let $H \subseteq V$ be such that $G[H]$ is $\chi(G[H])$-critical and $\overline{G}[H]$ is connected. Once again, in order to show that inequality (5) is facet defining, we are concerned with solutions to the linear system $\lambda x = \beta$, but this time over colorings x that satisfy (5) at equality. For each case that occurs in the proof, we proceed by choosing a coloring $\mathcal{S} = \{S_1, \ldots, S_k\}$ of G using $k \geqslant \chi(G)$ colors such that $S_1, \ldots, S_{\chi(G[H])}$ is a cover of H. Once such a coloring is chosen, we take as its incidence vector a $X^{\mathcal{S}}$ such that the representative of S_i is some vertex in H if and only if $i \in \{1, \ldots, \chi(G[H])\}$. This choice of $X^{\mathcal{S}}$ satisfies (5) at equality.

To show the zero entries of λ, there are two cases. In the first case, we take two anti-neighbors u and v such that $u \in H$ or $v \notin H$ and show that $\lambda_{uv} = 0$. The coloring $\mathcal{S}$ chosen in this case is such that $S_i = \{u\}$, for some $i \in \{1, \ldots, k\}$. The existence of such a coloring is guaranteed by two facts. First, if $u \in H$, then $G[H-u]$ can be colored with $\chi(G[H]) - 1$ colors because $G[H]$ is $\chi(G[H])$-critical. Second, if $u \notin H$, then we can take k as large as necessary to accommodate $\{u\}$ in $\mathcal{S}$. The desired result follows since $X^{\mathcal{S}} + x^{uv}$ also satisfies (5) at equality. For the second case, we assume that $v \in V \setminus H$, and we need to show that $\lambda_{vv} = 0$. By Assumption 1, v has an anti-neighbor u. Hence, we choose an $\mathcal{S}$ that includes the color class $\{u, v\}$, with u representing v. The existence of such an $\mathcal{S}$ stems from the same argument as before. Thus, $X^{\mathcal{S}} + x^{vv}$ satisfies (5) at equality and leads to $\lambda_{vv} = 0$, as required.

For the non-zero entries of λ, initially we show that if $v \in H$ and $uv \notin E$, then both $\lambda_{vv} = \lambda_{uv}$ and $\lambda_{vv} = \lambda_{uu}$, respectively if $u \notin H$ and $u \in H$. Again because $G[H]$ is $\chi(G[H])$-critical, we choose the coloring $\mathcal{S}$ containing $\{u, v\}$ and having v as its representative, no matter u belongs to H or not. Then, $X^{\mathcal{S}}$ and $X^{\mathcal{S}} - x^{vv} - x^{vu} + x^{uu} + x^{uv}$ satisfy (5) at equality. Once $\lambda_{vu} = 0$, due to $v \in H$, the desired results follow by using these vectors and recalling that $\lambda_{uu} = 0$, if $u \notin H$, and $\lambda_{uv} = 0$, otherwise. Finally, suppose $u, v \in H$ and $uv \in E$. It follows from the connectivity of $\overline{G}[H]$ that there exists a path $u = v_1, \ldots, v_\ell = v$ in $\overline{G}[H]$, leading to

$$\lambda_{uu} = \lambda_{v_1 v_1} = \cdots = \lambda_{v_\ell v_\ell} = \lambda_{vv}.$$

This shows that $\lambda_{vv} = \lambda_{uu}$, for all $u, v \in H$, concluding the proof for the non-zero entries of λ. This also concludes the proof of the theorem. □

It should be noted that, if $G[H]$ is $\chi(G[H])$-critical and $\overline{G}[H]$ is disconnected, then inequality (5) is not facet defining. For, let $H_1, \ldots, H_\ell$, $\ell > 1$, be the subsets of H inducing the connected components of $\overline{G}[H]$. It turns out that every independent set of $G[H]$ intersects only one H_i. Thus, each $G[H_i]$ is $\chi(G[H_i])$-critical and $\chi(G[H]) = \sum_{i=1}^{\ell} \chi(G[H_i])$. This means that (5) is the summation of the $\chi(G[H_i])$-critical inequalities, for all $i = 1, \ldots, \ell$.

Corollary 9. *If $G[H]$ is an odd hole or anti-hole, then* (5) *is facet defining for $P(G)$.*

Proof. If $G[H]$ is an odd hole or anti-hole, then it is 3- or $(|H|+1)/2$-critical, respectively [1]. Moreover, $\overline{G}[H]$ is clearly connected in both cases. □

4. Concluding remarks

One major difficulty in solving the vertex coloring problem on a given graph is to appropriately color its induced maximal cliques, odd holes and odd anti-holes. It is natural, then, that these structures play a central role when characterizing optimal colorings. In this context, we proposed a new 0–1 integer programming formulation of the vertex coloring problem and we showed that the aforementioned structures induce facets of the associated polytope. This formulation is simpler and more compact than other formulations in the literature. In particular, it can be seen as a variation of the MIS formulation that uses only $\mathrm{O}(n + \overline{m})$ binary variables to represent the independent sets of the graph. However, at the same time that this formulation is more compact, it presents some symmetry since there exist $|S|$ different assignments to the variables that represent an arbitrary independent set S. This is not alarming because establishing an order on the vertices beforehand, which also defines an order on the different representations of each independent set, makes it possible to distinguish a single variable assignment to represent S. This astuteness breaks the symmetry of the formulation. Some problems remain open, though, when one thinks about efficient implementations using this formulation. The most intriguing being related to the design of effective heuristics to tackle the separation problem related to the maximal cliques and, mainly, to the induced odd holes and anti-holes.

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