ALGEBRAIC CHARACTERIZATION OF UNIQUELY VERTEX COLORABLE GRAPHS

CHRISTOPHER J. HILLAR AND TROELS WINDFELDT

ABSTRACT. The study of graph vertex colorability from an algebraic perspective has introduced novel techniques and algorithms into the field. For instance, k-colorability of a graph can be characterized in terms of whether its graph polynomial is contained in a certain ideal. In this paper, we interpret unique colorability in an analogous manner and use Gröbner basis techniques to prove an algebraic characterization for uniquely k-colorable graphs. Our result also gives algorithms for testing unique colorability. As an application, we verify a counterexample to a conjecture of Xu concerning uniquely 3-colorable graphs without triangles.

1. Introduction

Let G be a simple, undirected graph with vertices $V = \{1, ..., n\}$ and edges E. The graph polynomial of G is given by

$$f_G = \prod_{\substack{\{i,j\} \in E, \\ i < j}} (x_i - x_j).$$

Fix a positive integer k < n, and let $C_k = \{c_1, \ldots, c_k\}$ be a k-element set. Each element of C_k is called a *color*. A (vertex) k-coloring of G is a map $\nu : V \to C_k$. We say that a k-coloring ν is proper if adjacent vertices receive different colors; otherwise ν is called *improper*. The graph G is said to be k-colorable if there exists a proper k-coloring of G.

Let k be an algebraically closed field of characteristic not dividing k, so that it contains k distinct kth roots of unity. Also, set $R = k[x_1, \ldots, x_n]$ to be the polynomial ring over k in indeterminates x_1, \ldots, x_n . Let \mathcal{H} be the set of graphs with vertices $\{1, \ldots, n\}$ consisting of a clique of size k+1 and isolated vertices. We will be interested in the following ideals of R:

$$J_{n,k} = \langle f_H : H \in \mathcal{H} \rangle,$$

$$I_{n,k} = \langle x_i^k - 1 : i \in V \rangle,$$

$$I_{G,k} = I_{n,k} + \langle x_i^{k-1} + x_i^{k-2} x_j + \dots + x_i x_j^{k-2} + x_j^{k-1} : \{i, j\} \in E \rangle.$$

One should think of $I_{n,k}$ and $I_{G,k}$ as representing the set of all k-colorings and proper k-colorings of the graph G, respectively. These ideals are important because

1

Key words and phrases. Vertex coloring, Gröbner basis, colorability algorithm, uniquely colorable graph.

The work of the first author is supported under a National Science Foundation Graduate Research Fellowship. This work was conducted during the Special Semester on Gröbner Bases, February 1 – July 31, 2006, organized by RICAM, Austrian Academy of Sciences, and RISC, Johannes Kepler University, Linz, Austria.

they allow for an algebraic formulation of k-colorability. The following theorem collects the results in the series of papers [3, 4, 12, 13, 14].

Theorem 1.1. The following four statements are equivalent:

- (1) The graph G is not k-colorable.
- (2) The constant polynomial 1 belongs to the ideal $I_{G,k}$.
- (3) The graph polynomial f_G belongs to the ideal $I_{n,k}$.
- (4) The graph polynomial f_G belongs to the ideal $J_{n,k}$.

The equivalence between (1) and (2) is due to Bayer [4] (see also chapter 2.7 of [1]). Alon and Tarsi [3] proved that (1) and (3) are equivalent, but also de Loera [12] and Mnuk [14] have proved this using Gröbner basis methods. Finally, the equivalence between (1) and (4) was proved by Kleitman and Lovász [13].

The next result says that the generators for the ideal $J_{n,k}$ in the above theorem are very special (see Section 2 for a review of the relevant definitions). A proof can be found in [12].

Theorem 1.2 (J. de Loera). The set of polynomials, $\{f_H : H \in \mathcal{H}\}$, is a universal Gröbner basis of $J_{n,k}$.

Remark 1.3. The set $\mathcal{G} = \{x_1^k - 1, \dots, x_n^k - 1\}$ is a universal Gröbner basis of $I_{n,k}$, but this follows easily since the leading terms of \mathcal{G} are relatively prime [7], regardless of term order.

We give a self-contained proof of Theorem 1.1 in Section 2. We say that a graph is uniquely k-colorable if there is a unique proper k-coloring up to permutation of the colors in C_k . In this case, partitions of the vertices into subsets having the same color are the same for each of the k! proper colorings of G. A natural refinement of Theorem 1.1 would be an algebraic characterization of when a k-colorable graph is uniquely k-colorable. Our main result provides such a characterization. To state the theorem, however, we need to introduce some notation.

Let G be a colorable graph with proper coloring ν , and let k be the number of distinct colors in $\nu(V)$. Then G is a k-colorable graph, which has a coloring using all k colors. The color class cl(i) of a vertex $i \in V$ is the set of vertices with the same color as i, and the representative of a color class is the largest vertex contained in it. We set $m_1 < m_2 < \cdots < m_k = n$ to be the representatives of the k color classes.

For a subset $U \subseteq V$ of the vertices, let h_U^d be the sum of all monomials of degree d in the indeterminates $\{x_i : i \in U\}$. We also set $h_U^0 = 1$. For each vertex $i \in V$, define a polynomial g_i as follows:

(1.1)
$$g_{i} = \begin{cases} x_{i}^{k} - 1 & \text{if } i = m_{k}, \\ h_{\{m_{j}, \dots, m_{k}\}}^{j} & \text{if } i = m_{j} \text{ for some } j \neq k, \\ h_{\{i, m_{2}, \dots, m_{k}\}}^{1} & \text{if } i \in cl(m_{1}), \\ x_{i} - x_{\max cl(i)} & \text{otherwise.} \end{cases}$$

A concrete instance of this construction may be found in Example 1.7 below. There is also a single polynomial g that is in some sense "dual" to the set of g_i ; however, we postpone a definition until Section 4.

Remark 1.4. It is easy to see that the map $\nu \mapsto \{g_1, \ldots, g_n\}$ depends only on how ν partitions V into color classes cl(i). In particular, if G is uniquely k-colorable, then there is a unique such set of polynomials $\{g_1, \ldots, g_n\}$ that corresponds to G.

We may now state our main theorem.

Theorem 1.5. Suppose ν is a k-coloring of G that uses all k colors, and let g_1, \ldots, g_n be given by (1.1) and g by (4.6). Then the following three statements are equivalent:

- (1) The graph G is uniquely k-colorable.
- (2) The polynomials g_1, \ldots, g_n belong to the ideal $I_{G,k}$.
- (3) The graph polynomial f_G belongs to the ideal $I_{n,k} + \langle g \rangle$.

For a uniquely colorable graph, the polynomials g_1, \ldots, g_n in the theorem do not depend on ν . In this case, there is a partial analog to Theorem 1.2 that refines Theorem 1.5. This result also gives us an algorithm for determining unique k-colorability that is independent of the knowledge of a coloring.

Theorem 1.6. A graph G is uniquely k-colorable if and only if the reduced Gröbner basis for $I_{G,k}$ with respect to the lexicographic order with $x_n \prec \cdots \prec x_1$ has the form $\{g_1,\ldots,g_n\}$ for polynomials as in (1.1).

Example 1.7. We present an example of a uniquely 3-colorable graph on n=12 vertices and give the polynomials g_1, \ldots, g_n from Theorem 1.5.

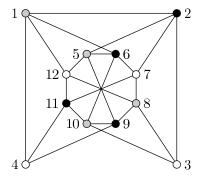


FIGURE 1. A uniquely 3-colorable graph without triangles [6].

Let G be the graph given in Figure 1. The indicated 3-coloring partitions V into the color classes $(m_1, m_2, m_3) = (10, 11, 12)$. The following set of 12 polynomials is the reduced Gröbner basis for the ideal $I_{G,k}$ with respect to the lexicographic ordering with $x_{12} \prec \cdots \prec x_1$. The leading terms of each g_i are underlined.

$$\begin{aligned} &\{\underline{x_{12}^3} - 1,\, \underline{x_7} - x_{12},\, \underline{x_4} - x_{12},\, \underline{x_3} - x_{12},\\ &\underline{x_{11}^2} + x_{11}x_{12} + x_{12}^2,\, \underline{x_9} - x_{11},\, \underline{x_6} - x_{11},\, \underline{x_2} - x_{11},\\ &\underline{x_{10}} + x_{11} + x_{12},\, \underline{x_8} + x_{11} + x_{12},\, \underline{x_5} + x_{11} + x_{12},\, \underline{x_1} + x_{11} + x_{12}\}. \end{aligned}$$

Notice that the leading terms of the polynomials in each line above correspond to the different color classes of this coloring of G.

The organization of this paper is as follows. In Section 2, we discuss some of the algebraic tools that will go into the proofs of our main results. Section 3 is devoted to a proof of Theorem 1.1, and in Section 4, we present arguments for Theorems 1.5 and 1.6. Theorems 1.1 and 1.5 give algorithms for testing k-colorability and unique

k-colorability of graphs, and we discuss the implementation of them in Section 5, along with a verification of a counterexample [2] to a conjecture [6, 9, 15] by Xu.

2. Algebraic Preliminaries

We briefly review the basic concepts of commutative algebra that will be useful for us here. Let I be an ideal of $R = \mathbb{k}[x_1, \dots, x_n]$. The variety V(I) of I is the set of points in \mathbb{k}^n that are zeroes of all the polynomials in I. Conversely, the vanishing ideal I(V) of a set $V \subseteq \mathbb{k}^n$ is the ideal of those polynomials vanishing on all of V. These two definitions are related by way of V(I(V)) = V and $I(V(I)) = \sqrt{I}$, in which

$$\sqrt{I} = \{f : f^n \in I \text{ for some } n\}$$

is the radical of I. The ideal I is called zero-dimensional if V(I) is finite. A term order \prec for the monomials of R is a well-ordering which is multiplicative and for which the constant monomial 1 is smallest. The initial term (or leading monomial) $in_{\prec}(f)$ of a polynomial $f \in R$ is the largest monomial in f with respect to \prec . The standard monomials $\mathcal{B}_{\prec}(I)$ of I are those monomials which are not the leading monomials of any polynomial in I.

Many arguments in commutative algebra and algebraic geometry are simplified when restricted to radical, zero-dimensional ideals (resp. multiplicity-free, finite varieties), and those found in this paper are not exceptions. The following fact is useful in this regard.

Lemma 2.1. Let I be a zero-dimensional ideal and fix a term order \prec . Then $\dim_{\mathbb{K}} R/I = |\mathcal{B}_{\prec}(I)| \geq |V(I)|$. Furthermore, the following are equivalent:

- (1) I is a radical ideal.
- (2) I contains a univariate square-free polynomial in each indeterminate.
- (3) $|\mathcal{B}_{\prec}(I)| = |V(I)|$.

Proof. See
$$[7]$$
.

A finite subset \mathcal{G} of an ideal I is a *Gröbner basis* (with respect to \prec) if the *initial ideal*,

$$in_{\prec}(I) = \langle in_{\prec}(f) : f \in I \rangle,$$

is generated by the initial terms of elements of \mathcal{G} . Furthermore, a universal Gröbner basis is a set of polynomials which is a Gröbner basis with respect to all term orders. The fundamental concepts of Gröbner bases were introduced by Buchberger [5] in his Ph.D. thesis. Many of the properties of I and V(I) can be calculated by finding a Gröbner basis for I, and such generating sets are fundamental for computation (including the algorithms presented in the last section).

Finally, a useful operation on two ideals I and J is the construction of the *colon ideal* $I: J = \{h \in R : hJ \subseteq I\}$. If V and W are two varieties, then the colon ideal

$$(2.1) I(V): I(W) = I(V \setminus W)$$

corresponds to a set difference.

3. Vertex Colorability

In what follows, the set of colors C_k will be the set of kth roots of unity, and we will freely speak of points in \mathbb{k}^n with all coordinates in C_k as colorings of G. In this case, a point $(v_1, \ldots, v_n) \in \mathbb{k}^n$ corresponds to a coloring of vertex i with color v_i for $i = 1, \ldots, n$. The varieties corresponding to the ideals $I_{n,k}$, $I_{G,k}$, and $I_{n,k} + \langle f_G \rangle$ partition the k-colorings of G as follows.

Lemma 3.1. The varieties $V(I_{n,k})$, $V(I_{G,k})$, and $V(I_{n,k} + \langle f_G \rangle)$ are in bijection with all, the proper, and the improper k-colorings of G, respectively.

Proof. The points in $V(I_{n,k})$ are all *n*-tuples of *k*th roots of unity and therefore naturally correspond to all *k*-colorings of *G*. Let $\mathbf{v} = (v_1, \ldots, v_n) \in V(I_{G,k})$; we must show that it corresponds to a proper coloring of *G*. Let $\{i, j\} \in E$ and set

$$q_{ij} = \frac{x_i^k - x_j^k}{x_i - x_j} \in I_{G,k}.$$

If $v_i = v_j$, then $q_{ij}(\mathbf{v}) = kv_i^{k-1} \neq 0$. Thus, the coloring \mathbf{v} is proper. Conversely, suppose that $\mathbf{v} = (v_1, \dots, v_n)$ is a proper coloring of G. Then, since

$$q_{ij}(\mathbf{v})(v_i - v_j) = (v_i^k - v_j^k) = 1 - 1 = 0,$$

it follows that for $\{i, j\} \in E$, we have $q_{ij}(\mathbf{v}) = 0$. This shows that $\mathbf{v} \in V(I_{G,k})$. Finally, if \mathbf{v} is an improper coloring, then it is easy to see that $f_G(\mathbf{v}) = 0$, and that moreover, any $\mathbf{v} \in V(I_{n,k})$ for which $f_G(\mathbf{v}) = 0$ has two coordinates, corresponding to an edge in G, that are equal.

The next result follows directly from Lemma 2.1. It will prove useful in simplifying many of the proofs in this paper.

Lemma 3.2. The ideals $I_{n,k}$, $I_{G,k}$, and $I_{n,k} + \langle f_G \rangle$ are radical.

We next describe a relationship between $I_{n,k}$, $I_{G,k}$, and $I_{n,k} + \langle f_G \rangle$.

Lemma 3.3. $I_{n,k} : I_{G,k} = I_{n,k} + \langle f_G \rangle$.

Proof. Let V and W be the set of all colorings and proper colorings, respectively, of the graph G. Now apply Lemma 3.1 and Lemma 3.2 to equation (2.1).

The dimensions of the residue rings corresponding to these ideals are readily computed from the above discussion. Recall that the *chromatic polynomial* χ_G is the univariate polynomial for which $\chi_G(k)$ is the number of proper k-colorings of G

Lemma 3.4. Let χ_G be the chromatic polynomial of G. Then

$$\chi_G(k) = \dim_{\mathbb{K}} R/I_{G,k},$$

$$k^n - \chi_G(k) = \dim_{\mathbb{K}} R/(I_{n,k} + \langle f_G \rangle).$$

Proof. Both equalities follow from Lemmas 2.1 and 3.1.

Let $K_{n,k}$ be the ideal of all polynomials $f \in R$ such that $f(v_1, \ldots, v_n) = 0$, $(v_1, \ldots, v_n) \in \mathbb{k}^n$, if at most k of the v_i are distinct. Clearly, $J_{n,k} \subseteq K_{n,k}$. We will need the following result of Kleitman and Lovász [13].

Theorem 3.5. The ideals $K_{n,k}$ and $J_{n,k}$ are the same.

Proof. We sketch the proof (see [13] for more details). Let $f \in K_{n,k}$ and for each subset $S \subseteq \{1, \ldots, n-1\}$, let f_S be the polynomial gotten from substituting x_n for each x_i with $i \in S$. Since $f_S \in K_{n,k}$, induction on the number of indeterminates n implies that $f_S \in J_{n,k}$ for nonempty S. If $p = x_1^{a_1} \cdots x_n^{a_n}$ is a monomial, then

$$q(p) := \sum_{S} (-1)^{|S|} p_S, \quad p \in R,$$

equals $(x_1^{a_1}-x_n^{a_1})\cdots(x_{n-1}^{a_{n-1}}-x_n^{a_{n-1}})x_n^{a_n}$. By linearity, therefore, it follows that $q=q(f)=(x_1-x_n)\cdots(x_{n-1}-x_n)h$ for some $h\in R$. Since $q\in K_{n,k}$, the polynomial h is zero whenever at most k-1 of the x_1,\ldots,x_{n-1} are distinct. Thus, upon expanding h in terms of powers of x_n , the coefficients will belong to $K_{n-1,k-1}$, and by induction, we may assume they all belong to $J_{n-1,k-1}$. Hence, $q\in J_{n,k}$. Finally, we have $f=q-\sum_{S\neq\emptyset}(-1)^{|S|}f_S\in J_{n,k}$, completing the proof.

We now present a proof of Theorem 1.1.

Proof of Theorem 1.1. (1) \Rightarrow (2): Suppose that G is not k-colorable. Then it follows from Lemma 3.4 that $\dim_{\mathbb{K}} R/I_{G,k} = 0$ and so $1 \in I_G$. (2) \Rightarrow (3): Suppose that $I_{G,k} = \langle 1 \rangle$ so that $I_{n,k} : I_{G,k} = I_{n,k}$. Then Lemma 3.3 implies that $I_{n,k} + \langle f_G \rangle = I_{n,k}$ and hence $f_G \in I_{n,k}$. (3) \Rightarrow (1): Assume that f_G belongs to the ideal $I_{n,k}$. Then $I_{n,k} + \langle f_G \rangle = I_{n,k}$, and it follows from Lemma 3.4 that $k^n - \chi_G(k) = k^n$. Therefore, $\chi_G(k) = 0$ as desired. (4) \Rightarrow (1): Suppose that $f_G \in J_{n,k}$. Then from Theorem 3.5, there can be no proper coloring \mathbf{v} (there are at most k distinct coordinates). (1) \Rightarrow (4): If G is not k-colorable, then for every substitution $\mathbf{v} \in \mathbb{k}^n$ with at most k distinct coordinates, we must have $f_G(\mathbf{v}) = 0$. It follows that $f_G \in J_{n,k}$ from Theorem 3.5.

4. Unique Vertex Colorability

Let G be a colorable graph with proper coloring ν , and let k be the number of distinct colors in $\nu(V)$. For each vertex $i \in V$, we assign a polynomial g_i as in equation (1.1) from the introduction. One should think (loosely) of the first case of (1.1) as corresponding to a choice of a color for the last vertex; the second and third, to subsets of vertices in different color classes; and the fourth, to the fact that elements in the same color class should have the same color. These polynomials encode the coloring ν algebraically in a computationally useful way (see Lemmas 4.1 and 4.3 below).

Recall that a reduced Gröbner basis \mathcal{G} is a Gröbner basis such that (1) the coefficient of $in_{\prec}(g)$ for each $g \in \mathcal{G}$ is 1 and (2) the leading monomial of any $g \in \mathcal{G}$ does not divide any monomial occurring in another polynomial in \mathcal{G} . Given a term order, reduced Gröbner bases exist and are unique.

Lemma 4.1. Let \prec be the lexicographic ordering induced by $x_n \prec \cdots \prec x_1$. Then the set of polynomials $\{g_1, \ldots, g_n\}$ is the reduced Gröbner basis with respect to \prec for the ideal it generates.

Proof. It is clear by construction that the initial terms of $\{g_1, \ldots, g_n\}$ are relatively prime. It follows that these polynomials form a Gröbner basis for the ideal they generate (again from [7]). That they are reduced also follows by inspection of (1.1).

The following innocuous-looking fact is a very important ingredient in the proof of Theorem 1.5.

Lemma 4.2. Let U be a subset of $\{1, \ldots, n\}$, and suppose that $\{i, j\} \subseteq U$. Then

$$(4.1) (x_i - x_j)h_U^d = h_{U \setminus \{j\}}^{d+1} - h_{U \setminus \{i\}}^{d+1},$$

for all nonnegative integers d.

Proof. We induct on the number of elements in U. When $U = \{i, j\}$, the relation is clear from

$$h_{\{i,j\}}^d = \frac{x_i^{d+1} - x_j^{d+1}}{x_i - x_j}.$$

Suppose now that U has at least three elements and let $l \in U$ be different from i and j. Then,

$$(x_{i} - x_{j})h_{U}^{d} = (x_{i} - x_{j}) \sum_{r=0}^{d} x_{l}^{r} h_{U \setminus \{l\}}^{d-r}$$

$$= \sum_{r=0}^{d} x_{l}^{r} (x_{i} - x_{j}) h_{U \setminus \{l\}}^{d-r}$$

$$= \sum_{r=0}^{d} x_{l}^{r} \left(h_{U \setminus \{j,l\}}^{d+1-r} - h_{U \setminus \{i,l\}}^{d+1-r} \right)$$

$$= \sum_{r=0}^{d} x_{l}^{r} h_{U \setminus \{j,l\}}^{d+1-r} - \sum_{r=0}^{d} x_{l}^{r} h_{U \setminus \{i,l\}}^{d+1-r}$$

$$= \left(h_{U \setminus \{j\}}^{d+1} - x_{l}^{d+1} \right) - \left(h_{U \setminus \{i\}}^{d+1} - x_{l}^{d+1} \right)$$

$$= h_{U \setminus \{j\}}^{d+1} - h_{U \setminus \{i\}}^{d+1}.$$

This completes the induction and the proof.

That the polynomials g_1, \ldots, g_n represent an algebraic encoding of the coloring ν is explained by the following technical lemma.

Lemma 4.3. Let g_1, \ldots, g_n be given as in (1.1). Then the following three properties hold for the ideal $A = \langle g_1, \ldots, g_n \rangle$:

- (1) $I_{G,k} \subseteq A$,
- (2) A is radical,
- (3) |V(A)| = k!.

Proof. First assume that $I_{G,k} \subseteq A$. Then A is radical from Lemma 2.1. Moreover, since the polynomials $\{g_1, \ldots, g_n\}$ form a Gröbner basis for the ideal A, the number of standard monomials of A is equal to |V(A)|. By inspection of (1.1) using the ordering in Lemma 4.1, we have $|\mathcal{B}_{\prec}(A)| = k!$, and therefore (3) is proved.

We now prove statement (1). First, we give explicit representations of polynomials $x_i^k - 1 \in I_{n,k}$ in terms of the generators of A. We first claim that for $i = 1, \ldots, k$, we have

(4.2)
$$x_{m_i}^k - 1 = x_n^k - 1 + \sum_{l=i}^{k-1} \left[\prod_{j=l+1}^k \left(x_{m_i} - x_{m_j} \right) \right] h_{\{m_l, \dots, m_k\}}^l.$$

To verify (4.2) for a fixed i, we will use Lemma 4.2 and induction to prove that for each positive integer $s \leq k - i$, the sum on the right hand-side above is equal to

$$(4.3) \prod_{j=s+i}^{k} \left(x_{m_i} - x_{m_j} \right) h_{\{m_i, m_{s+i}, \dots, m_k\}}^{s+i-1} + \sum_{l=s+i}^{k-1} \left[\prod_{j=l+1}^{k} \left(x_{m_i} - x_{m_j} \right) \right] h_{\{m_l, \dots, m_k\}}^{l}.$$

For s = 1, this is clear as (4.3) is exactly the sum on the right-hand side of (4.2). In general, using Lemma 4.2, the first term on the left hand side of (4.3) is

$$\prod_{j=s+i+1}^{k} \left(x_{m_i} - x_{m_j} \right) \left(h_{\{m_i, m_{s+1+i}, \dots, m_k\}}^{s+i} - h_{\{m_{s+i}, \dots, m_k\}}^{s+i} \right),$$

which is easily seen to cancel the first summand in the sum found in (4.3). Now, equation (4.3) with s = k - i gives us that the right hand side of (4.2) is

$$x_n^k - 1 + (x_{m_i} - x_{m_k})h_{\{m_i, m_k\}}^{k-1} = x_n^k - 1 + x_{m_i}^k - x_n^k = x_{m_i}^k - 1,$$

proving the claim. It follows that $x_i^k - 1 \in A$ when $i \in \{m_1, \dots, m_k\}$.

It remains to show that $x_i^k - 1 \in A$ for all i not in $\{m_1, \ldots, m_k\}$. For this, we first verify that $x_i - x_{m_i} \in A$. For those i not in the color class of vertex m_1 , this is clear from (1.1). Otherwise,

$$g_i - g_{m_1} = h^1_{\{i, m_2, \dots, m_k\}} - h^1_{\{m_1, \dots, m_k\}} = x_i - x_{m_1} \in A,$$

as desired. Let $f_i = x_i - x_{m_i}$ and notice that

$$x_{m_i}^k - 1 = (x_i - f_i)^k - 1 = x_i^k - 1 + f_i h \in A$$

for some polynomial h. It follows that $x_i^k - 1 \in A$.

Finally, we must verify that the other generators of $I_{G,k}$ are in A. To accomplish this, we will prove the following stronger statement:

$$(4.4) U \subseteq \{m_1, \dots, m_k\} \text{ with } |U| \ge 2 \implies h_U^{k+1-|U|} \in A.$$

We downward induct on s=|U|. In the case s=k, we have $U=\{m_1,\ldots,m_k\}$. But then as is easily checked $g_{m_1}=h_U^{k+1-|U|}\in A$. For the general case, we will show that if one polynomial $h_U^{k+1-|U|}$ is in A, with |U|=s< k, then $h_U^{k+1-|U|}\in A$ for any subset $U\subseteq \{m_1,\ldots,m_k\}$ of cardinality s. In this regard, suppose that $h_U^{k+1-|U|}\in A$ for a subset U with |U|=s< k. Let $u\in U$ and $v\in \{m_1,\ldots,m_k\}\setminus U$, and examine the following equality (using Lemma 4.2):

$$(x_u-x_v)h_{\{v\}\cup U}^{k-s}=h_U^{k-s+1}-h_{\{v\}\cup U\backslash \{u\}}^{k-s+1}.$$

By induction, the left hand side of this equation is in A and therefore the assumption on U implies that

$$h_{\{v\}\cup U\backslash\{u\}}^{k-s+1}\in A.$$

This shows that we may replace any element of U with any element of $\{m_1, \ldots, m_k\}$. Since there is a subset U of size s with $h_U^{k+1-|U|} \in A$ (see (1.1)), it follows from this that we have $h_U^{k+1-|U|} \in A$ for any subset U of size s. This completes the induction.

A similar trick as before using polynomials $x_i - x_{m_i} \in A$ proves that we may replace in (4.4) the requirement that $U \subseteq \{m_1, \ldots, m_k\}$ with one that says that U consists of vertices in different color classes. If $\{i, j\} \in E$, then i and j are

in different color classes, and therefore the generator $h_{\{i,j\}}^{k-1} \in I_{G,k}$ is in A. This finishes the proof of the lemma.

Remark 4.4. Property (1) in the lemma says that V(A) contains proper colorings of G while properties (2) and (3) say that, up to permutation of the colors, the zeroes of the polynomials g_1, \ldots, g_n correspond to the single proper coloring given by ν .

Lemma 4.5. Suppose that G is uniquely k-colorable. Then the following two statements hold:

- (1) If $\{i, j\} \subseteq V$ have the same color, then $x_i x_j \in I_{G,k}$.
- (2) If $U \subseteq V$ is a set with $|U| \ge 2$ consisting of vertices with all different colors, then $h_U^{k+1-|U|} \in I_{G,k}$.

Proof. Let $\mathbf{v} = (v_1, \dots, v_n) \in V(I_{G,k})$, which by Lemma 3.1 corresponds to a proper coloring. Since G is uniquely k-colorable, it follows that $v_i - v_j = 0$ for each i and j in the same color class. Thus $x_i - x_j \in I(V(I_{G,k})) = I_{G,k}$ since $I_{G,k}$ is radical. To prove the second statement, we induct on the size of U. Suppose that $U = \{i, j\}$ consists of two vertices with different colors, and let $\mathbf{v} = (v_1, \dots, v_n) \in V(I_{G,k})$. Then by Lemma 4.2,

$$(v_i - v_j)h_U^{k+1-|U|}(\mathbf{v}) = h_{U\setminus\{j\}}^k(\mathbf{v}) - h_{U\setminus\{i\}}^k(\mathbf{v}) = v_i^k - v_j^k = 0.$$

Since $v_i \neq v_j$, it follows that $h_U^{k+1-|U|} \in I_{G,k}$ in this case (using as before that $I_{G,k}$ is radical). For |U| > 2, we have,

$$(v_i - v_j)h_U^{k+1-|U|}(\mathbf{v}) = h_{U\setminus\{j\}}^{k+1-|U\setminus\{j\}|}(\mathbf{v}) - h_{U\setminus\{i\}}^{k+1-|U\setminus\{i\}|}(\mathbf{v}) = 0 - 0 = 0,$$

by Lemma 4.2 and the induction hypothesis. Again, it follows that $h_U^{k+1-|U|}(\mathbf{v}) = 0$, completing the induction and the proof.

Before proving our main theorem, we define the g in Theorem 1.5 using a "dual" set of auxiliary polynomials $\overline{g}_1, \ldots, \overline{g}_n$. Given a subset $U \subseteq V$ of the vertices of G, we let K_U denote the graph on vertices V with a clique on vertices U and isolated other vertices. For $i = 1, \ldots, n$, set

$$\overline{g}_{i} = \begin{cases} 1 & \text{if } i = m_{k}, \\ f_{K_{\{m_{j},...,m_{k}\}}} & \text{if } i = m_{j} \text{ for some } j \neq k, \\ f_{K_{\{i,m_{2},...,m_{k}\}}} & \text{if } i \in cl(m_{1}), \\ h_{\{i,\max{cl(i)}\}}^{k-1} & \text{otherwise.} \end{cases}$$

We can now define

$$(4.6) g = \overline{g}_1 \cdots \overline{g}_n.$$

The following is a duality relationship between g_1, \ldots, g_n and g.

Lemma 4.6.
$$I_{n,k}:\langle g_1,\ldots,g_n\rangle=I_{n,k}+\langle g\rangle$$
.

Proof. Since all the ideals in consideration are radical by Lemmas 2.1 and 4.3, equation (2.1) says that we need to show that

$$V(I_{n,k} + \langle g \rangle) = V(I_{n,k}) \backslash V(\langle g_1, \dots, g_n \rangle).$$

First, suppose that $\mathbf{v} = (v_1, \dots, v_n)$ is contained in the left-hand side of the above equation; we will verify it is in the right-hand side. In this case, $\overline{q}_i(\mathbf{v}) = 0$ for some

i. Suppose that i arises from the fourth case of (4.5), and let j be such that $m_j = \max cl(i)$. If $v_i = v_{m_j}$, then $h_{\{i,m_j\}}^{k-1}(\mathbf{v}) = kv_i^{k-1} \neq 0$, a contradiction. It follows that $v_i \neq v_{m_j}$, and therefore $\mathbf{v} \notin V(\langle g_1, \dots, g_n \rangle)$. If i comes from cases two or three in (4.5), then $\overline{g}_i(\mathbf{v}) = 0$ says that two coordinates of \mathbf{v} that represent vertices in different color classes are equal. But then this point cannot be in $V(\langle g_1, \dots, g_n \rangle)$ by Lemma 4.3 (specifically, Remark 4.4).

Conversely, suppose that \mathbf{v} is a coloring not contained in $V(\langle g_1,\ldots,g_n\rangle)$. Then $g_i(\mathbf{v})\neq 0$ for some i. This i cannot come from the first case of (1.1). If it arises from the fourth case, then $v_i-v_{m_j}\neq 0$ for some j. Thus, the equality $(v_i-v_{m_j})h_{\{i,m_j\}}^{k-1}(\mathbf{v})=v_i^k-v_{m_j}^k=0$ implies that $\overline{g}_i(\mathbf{v})=0$, as desired. Finally, suppose that $g_i(\mathbf{v})\neq 0$ for i from cases two or three, and let $S=\{i,m_2,\ldots,m_k\}$ or $S=\{m_j,\ldots,m_k\}$, respectively. Consider all subsets $U\subseteq S$ with at least 2 elements such that $h_U^{k+1-|U|}(\mathbf{v})\neq 0$ and choose one of minimum cardinality; this set exists by assumption. If $U=\{i,j\}$, then $(v_i-v_j)h_U^{k+1-|U|}(\mathbf{v})=v_i^k-v_j^k=0$ so that $v_i=v_j$ and $\overline{g}_i(\mathbf{v})=0$. Otherwise, if $\{i,j\}\subseteq U$, then

$$(v_i - v_j)h_U^{k+1-|U|}(\mathbf{v}) = h_{U\setminus\{j\}}^{k+1-|U\setminus\{j\}|}(\mathbf{v}) - h_{U\setminus\{i\}}^{k+1-|U\setminus\{i\}|}(\mathbf{v}) = 0,$$

by Lemma 4.2 and the minimality of U. Again, it follows that $v_i = v_j$ and $\overline{g}_i(\mathbf{v}) = 0$. Therefore, in all cases, $\mathbf{v} \in V(I_{n,k} + \langle g \rangle)$. This finishes the proof.

We are now in a position to prove our main theorem.

Proof of Theorem 1.5. (1) \Rightarrow (2): Suppose the graph G is uniquely k-colorable and construct the set of g_i from (1.1); we will prove that $g_i \in I_{G,k}$ for each $i \in V$. By Lemma 4.5, polynomials of the form $x_i - x_{m_i}$ are in $I_{G,k}$, and by definition of $I_{G,k}$, we have $x_n^k - 1 \in I_{G,k}$. Finally, since the sets $U = \{m_j, \ldots, m_k\}$ and $V = \{i, m_2, \ldots, m_k\}$ consist of vertices with different colors, those g_i of the form h_U^j and h_V^1 are in $I_{G,k}$ again by Lemma 4.5.

 $(2) \Rightarrow (3)$: Suppose that $A = \langle g_1, \dots, g_n \rangle \subseteq I_{G,k}$. From Lemmas 3.3 and 4.6, we have

$$I_{n,k} + \langle f_G \rangle = I_{n,k} : I_{G,k} \subseteq I_{n,k} : A = I_{n,k} + \langle g \rangle.$$

This proves that $f_G \in I_{n,k} + \langle g \rangle$.

 $(3) \Rightarrow (1)$: Assume that $f_G \in I_{n,k} + \langle g \rangle$. Then,

$$I_{n,k}: I_{G,k} = I_{n,k} + \langle f_G \rangle \subseteq I_{n,k} + \langle g \rangle = I_{n,k}: A.$$

Applying Lemmas 2.1 and 4.3, we have

$$(4.7) k^n - k! = |V(I_{n,k}) \setminus V(A)| = |V(I_{n,k} : A)| \le |V(I_{n,k} : I_{G,k})| \le k^n - k!,$$

since the number of improper colorings is at most $k^n - k!$. It follows that equality holds throughout (4.7) so that the number of proper colorings is k!. Therefore, G is uniquely k-colorable, completing the proof.

Collecting the results of this section, we can now also prove Theorem 1.6 from the introduction.

Proof of Theorem 1.6. The only-if direction of the theorem follows from $(2) \Rightarrow (1)$ of Theorem 1.5. For the other implication, by Lemma 4.1, it is enough to show that $A = \langle g_1, \ldots, g_n \rangle = I_{G,k}$. From Lemma 4.3, we know that $I_{G,k} \subseteq A$, and the other inclusion is clear also from the equivalence of (1) and (2) in Theorem 1.5. \square

5. Algorithms and Xu's Conjecture

In this section we describe the algorithms implied by Theorems 1.1 and 1.5, and illustrate their usefulness by disproving a conjecture of Xu. First, from Theorem 1.1, we have the following methods for determining k-colorability.

Algorithm 5.1.

Input: A graph G with vertices $V = \{1, ..., n\}$ and edges E, and a positive integer k. Output: true if G is k-colorable; otherwise false.

Method 1:

- (1) Compute a Gröbner basis \mathcal{G} of $I_{G,k}$.
- (2) Compute the normal form of the constant polynomial 1 wrt. \mathcal{G} .
- (3) Return *false* if the normal form is zero; otherwise return *true*.

- $\begin{array}{ll} (1) \ \, \mathrm{Set} \,\, \mathcal{G} := \{x_i^k 1 : i \in V\}. \\ (2) \ \, \mathrm{Set} \,\, f := 1. \end{array}$
- (3) For $\{i, j\} \in E$:

Compute the normal form g of $(x_i - x_j)f$ wrt. \mathcal{G} , and set f := g.

(4) Return false if f is zero; otherwise return true.

Method 3:

- (1) Set $\mathcal{G} := \{f_H : H \in \mathcal{H}\}$, where \mathcal{H} is the set of graphs with vertices $\{1,\ldots,n\}$ consisting of a clique of size k+1 and isolated vertices.
- (2) Set f := 1.
- (3) For $\{i, j\} \in E$:

Compute the normal form g of $(x_i - x_j)f$ wrt. \mathcal{G} , and set f := g.

(4) Return false if f is zero; otherwise return true.

The analogue of this algorithm for unique colorability is given by Theorem 1.5.

Algorithm 5.2.

Input: A graph G with vertices $V = \{1, \dots, n\}$ and edges E, and a k-coloring of G. Output: true if G is uniquely k-colorable; otherwise false.

Method 1:

- (1) Compute a Gröbner basis \mathcal{G} of $I_{G,k}$.
- (2) For $i \in V$:

Compute the normal form of g_i wrt. \mathcal{G} .

Return *false* if the normal form is nonzero.

(3) Return *true*.

Method 2:

- (1) Compute a Gröbner basis \mathcal{G} of $I_{n,k} + \langle g \rangle$.
- (2) Set f := 1.
- (3) For $\{i, j\} \in E$:

Compute the normal form g of $(x_i - x_j)f$ wrt. \mathcal{G} , and set f := g.

(4) Return true if f is zero; otherwise return false.

Remark 5.3. Although Theorem 1.6 gives a method for determining unique colorability independent of a coloring of G, in practice, it is more efficient to find some Gröbner basis for $I_{G,k}$ and use criterion (2) in Theorem 1.5.

 $^{^{1}}$ Code that performs this calculation along with an implementation in SINGULAR 3.0 (http://www.singular.uni-kl.de) of the algorithms in this section can be found at http://www.math.tamu.edu/~chillar/.

In [15], Xu showed that if G is a uniquely k-colorable graph with |V| = n and |E| = m, then $m \ge (k-1)n - {k \choose 2}$, and this bound is best possible. He went on to conjecture that if G is uniquely k-colorable with |V| = n and $|E| = (k-1)n - {k \choose 2}$, then G contains a k-clique. In [2], this conjecture was shown to be false for k = 3 and |V| = 24 using the graph in Figure 2; however, the proof is somewhat complicated. We verified that this graph is indeed a counterexample to Xu's conjecture using Algorithm 5.2, Method 1. The computation requires approximately a half hour of processor time on a laptop PC with a 1.6 GHz Intel Pentium M processor and 1 GB of memory. The code can be downloaded from the link at the beginning of this section.

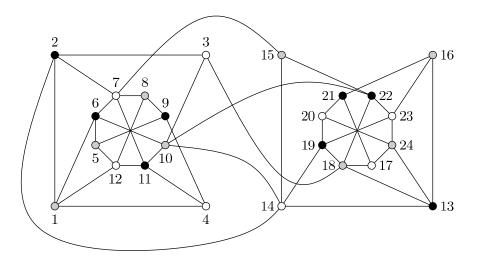


Figure 2. A counterexample to Xu's conjecture [2].

References

- [1] W. Adams, P. Loustaunau, An introduction to Grobner bases, AMS, 1994.
- [2] S. Akbari, V. S. Mirrokni, B. S. Sadjad, K_r -Free uniquely vertex colorable graphs with minimum possible edges. Journal of Combinatorial Theory, Series B 82 (2001), 316–318.
- [3] N. Alon, M. Tarsi, Colorings and orientations of graphs. Combinatorica 12 (1992), 125-134.
- [4] D. Bayer, The division algorithm and the Hilbert scheme. Ph.D. Thesis, Harvard University, 1982.
- [5] B. Buchberger, An algorithmic criterion for the solvability of algebraic systems of equations, Aequat. Math. 4 (1970), 374–383.
- [6] C.-Y. Chao, Z. Chen, On uniquely 3-colorable graphs. Discrete Mathematics 112 (1993), 21–27.
- [7] D. Cox, J. Little, D. O'Shea, Using algebraic geometry, Springer, New York, 1998.
- [8] D. Cox, J. Little, D. O'Shea, *Ideals, varieties, and algorithms*, Springer-Verlag, New York, 1997.
- [9] A. Daneshgar, R. Naserasr, On small uniquely vertex-colourable graphs and Xu's conjecture, Discrete Math. 223 (2000), 93–108.
- [10] F. Harary, S. T. Hedetniemi, R. W. Robinson, *Uniquely colorable graphs*, Journal of Combinatorial Theory 6 (1969), 264–270.
- [11] S.-Y. R. Li, W.-C. W. Li, Independence numbers of graphs and generators of ideals. Combinatorica 1 (1981), 55–61.

- [12] J. A. de Loera, Gröbner bases and graph colorings, Beitrage zur Algebra und Geometrie 36 (1995), 89-96.
- $[13] \ \text{L. Lov\'{a}sz}, \textit{Stable sets and polynomials}. \ \text{Discrete Mathematics } \textbf{124} \ (1994), \ 137-153.$
- [14] M. Mnuk, On an algebraic description of colorability of planar draphs. In Koji Nakagawa, editor, Logic, Mathematics and Computer Science: Interactions. Proceedings of the Symposium in Honor of Bruno Buchberger's 60th Birthday. RISC, Linz, Austria, October 20-22 (2002), 177-186.
- [15] S. Xu, The size of uniquely colorable graphs, Journal of Combinatorial Theory Series B 50 (1990), 319-320.

Department of Mathematics, Texas A&M University, College Station, TX 77843 $E ext{-}mail\ address: chillar@math.tamu.edu}$

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF COPENHAGEN, DENMARK. E-mail address: windfeldt@math.ku.dk