

# ALGEBRAIC CHARACTERIZATION OF UNIQUELY VERTEX COLORABLE GRAPHS

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ABSTRACT. The study of graph vertex colorability from an algebraic perspective has introduced novel techniques and algorithms into the field. For instance, it is known that  $k$ -colorability of a graph  $G$  is equivalent to the condition  $1 \notin I_{G,k}$  for a certain ideal  $I_{G,k} \subseteq \mathbb{k}[x_1, \dots, x_n]$ . In this paper, we extend this result by proving a general decomposition theorem for  $I_{G,k}$ . This theorem allows us to give an algebraic characterization of uniquely  $k$ -colorable graphs. Our results also give 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  $V = \{1, \dots, n\}$  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  $C_k = \{c_1, \dots, c_k\}$  be a  $k$ -element set. Each element of  $C_k$  is called a *color*. A (vertex)  $k$ -*coloring* of  $G$  is a map  $\nu : V \rightarrow C_k$ . We say that a  $k$ -coloring  $\nu$  is *proper* if adjacent vertices receive different colors; otherwise  $\nu$  is called *improper*. The graph  $G$  is said to be  $k$ -*colorable* if there exists a proper  $k$ -coloring of  $G$ .

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

$$\begin{aligned} J_{n,k} &= \langle f_H : H \in \mathcal{H} \rangle, \\ I_{n,k} &= \langle x_i^k - 1 : i \in V \rangle, \\ I_{G,k} &= I_{n,k} + \langle x_i^{k-1} + x_i^{k-2}x_j + \dots + x_i x_j^{k-2} + x_j^{k-1} : \{i, j\} \in E \rangle. \end{aligned}$$

One should think of (the zeroes of)  $I_{n,k}$  and  $I_{G,k}$  as representing  $k$ -colorings and proper  $k$ -colorings of the graph  $G$ , respectively (see Section 3). The idea of using roots of unity and ideal theory to study graph coloring problems seems to originate

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in Bayer's thesis [4], although it has appeared in many other places, including the work of de Loera [11] and Lovász [12]. These ideals are important because they allow for an algebraic formulation of  $k$ -colorability. The following theorem appears in the series of works [3, 4, 11, 12, 13].

**Theorem 1.1.** *The following statements are equivalent:*

- (1) *The graph  $G$  is not  $k$ -colorable.*
- (2)  $\dim_{\mathbb{k}} R/I_{G,k} = 0$ .
- (3) *The constant polynomial 1 belongs to the ideal  $I_{G,k}$ .*
- (4) *The graph polynomial  $f_G$  belongs to the ideal  $I_{n,k}$ .*
- (5) *The graph polynomial  $f_G$  belongs to the ideal  $J_{n,k}$ .*

The equivalence between (1) and (3) is due to Bayer [4, p. 109–112] (see also Chapter 2.7 of [1]). Alon and Tarsi [3] proved that (1) and (4) are equivalent, but also de Loera [11] and Mnuk [13] have proved this using Gröbner basis methods. The equivalence between (1) and (5) was proved by Kleitman and Lovász [12]. We give a self-contained and simplified proof of Theorem 1.1 in Section 2, in part to collect the many facts we need here.

The next result says that the generators for the ideal  $J_{n,k}$  in the above theorem are very special. A proof can be found in [11]. (In Section 2, we will review the relevant definitions regarding term orders and Gröbner bases).

**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, regardless of term order [1, Theorem 1.7.4 and Lemma 3.3.1].

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. We provide such a characterization. It will be a corollary to our main theorem (Theorem 1.7) that decomposes the ideal  $I_{G,k}$  into an intersection of simpler “coloring ideals”. To state the theorem, however, we need to introduce some notation.

Let  $\nu$  be a proper  $k$ -coloring of a graph  $G$ . Also, let  $l \leq k$  be the number of distinct colors in  $\nu(V)$ . The *color class*  $cl(i)$  of a vertex  $i \in V$  is the set of vertices with the same color as  $i$ , and the *maximum* of a color class is the largest vertex contained in it. We set  $m_1 < m_2 < \dots < m_l = n$  to be the maximums of the  $l$  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  $h_U^0 = 1$ .

**Definition 1.4** ( $\nu$ -bases). Let  $\nu$  be a proper  $k$ -coloring of a graph  $G$ . For each vertex  $i \in V$ , define a polynomial  $g_i$  as follows:

$$(1.1) \quad g_i = \begin{cases} x_i^k - 1 & \text{if } i = m_l, \\ h_{\{m_j, \dots, m_l\}}^{k-l+j} & \text{if } i = m_j \text{ for some } j \neq l, \\ x_i - x_{\max cl(i)} & \text{otherwise.} \end{cases}$$

The collection  $\{g_1, \dots, g_n\}$  is called a  $\nu$ -basis for the graph  $G$  with respect to the proper coloring  $\nu$ .

As we shall soon see, this set is a (minimal) Gröbner basis; its initial ideal is generated by the relatively prime monomials

$$\{x_{m_1}^{k-l+1}, x_{m_2}^{k-l+2}, \dots, x_{m_l}^k\} \text{ and } \{x_i : i \neq m_j \text{ for any } j\}.$$

A concrete instance of this construction may be found in Example 1.8 below.

*Remark 1.5.* It is easy to see that the map  $\nu \mapsto \{g_1, \dots, g_n\}$  depends only on how  $\nu$  partitions  $V$  into color classes  $cl(i)$ . In particular, if  $G$  is uniquely  $k$ -colorable, then there is a unique such set of polynomials  $\{g_1, \dots, g_n\}$  that corresponds to  $G$ .

This discussion prepares us to make the following definition.

**Definition 1.6** (Coloring Ideals). Let  $\nu$  be a proper  $k$ -coloring of a graph  $G$ . The  $k$ -coloring ideal (or simply *coloring ideal* if  $k$  is clear from the context) associated to  $\nu$  is the ideal

$$A_\nu = \langle g_1, \dots, g_n \rangle,$$

where the  $g_i$  are given by (1.1).

In a precise way to be made clear later (see Lemma 4.4), the coloring ideal associated to  $\nu$  algebraically encodes the proper  $k$ -coloring of  $G$  by  $\nu$  (up to relabeling of the colors). We may now state our main theorem.

**Theorem 1.7.** *Let  $G$  be a simple graph with  $n$  vertices. Then*

$$I_{G,k} = \bigcap_{\nu} A_\nu,$$

where  $\nu$  runs over all proper  $k$ -colorings of  $G$ .

*Example 1.8.* Let  $G = (\{1, 2, 3\}, \{\{1, 2\}, \{2, 3\}\})$  be the path graph on three vertices, and let  $k = 3$ . There are essentially two proper 3-colorings of  $G$ : the one where vertices 1 and 3 receive the same color, and the one where all the vertices receive different colors. If we denote by  $\nu_1$  the former, and by  $\nu_2$  the latter, then according to Definition 1.6, we have:

$$\begin{aligned} A_{\nu_1} &= \langle x_3^3 - 1, x_2^2 + x_2x_3 + x_3^2, x_1 - x_3 \rangle, \\ A_{\nu_2} &= \langle x_3^3 - 1, x_2^2 + x_2x_3 + x_3^2, x_1 + x_2 + x_3 \rangle. \end{aligned}$$

The intersection  $A_{\nu_1} \cap A_{\nu_2}$  is equal to the graph ideal,

$$I_{G,3} = \langle x_1^3 - 1, x_2^3 - 1, x_3^3 - 1, x_1^2 + x_1x_2 + x_2^2, x_2^2 + x_2x_3 + x_3^2 \rangle,$$

as predicted by Theorem 1.7.

Two interesting special cases of this theorem are the following. When  $G$  has no proper  $k$ -colorings, Theorem 1.7 says that  $I_{G,k} = \langle 1 \rangle$  in accordance with Theorem 1.1. And for a graph that is uniquely  $k$ -colorable, all of the ideals  $A_\nu$  are the same. This observation allows us to use Theorem 1.7 to give the following algebraic characterization of uniquely colorable graphs.

**Theorem 1.9.** *Suppose  $\nu$  is a  $k$ -coloring of  $G$  that uses all  $k$  colors, and let  $g_1, \dots, g_n$  be given by (1.1). Then the following statements are equivalent:*

- (1) *The graph  $G$  is uniquely  $k$ -colorable.*
- (2) *The polynomials  $g_1, \dots, g_n$  generate the ideal  $I_{G,k}$ .*

- (3) The polynomials  $g_1, \dots, g_n$  belong to the ideal  $I_{G,k}$ .
- (4) The graph polynomial  $f_G$  belongs to the ideal  $I_{n,k} : \langle g_1, \dots, g_n \rangle$ .
- (5)  $\dim_{\mathbb{k}} R/I_{G,k} = k!$ .

There is also a partial analogue to Theorem 1.2 that refines Theorem 1.9. This result gives us an algorithm for determining unique  $k$ -colorability that is independent of the knowledge of a proper coloring. To state it, we need only make a slight modification of the polynomials in (1.1). Suppose that  $\nu$  is a proper coloring with  $l = k$  (for instance, this holds when  $G$  is uniquely  $k$ -colorable). Then, for  $i \in V$  we define:

$$(1.2) \quad \tilde{g}_i = \begin{cases} x_i^k - 1 & \text{if } i = m_l, \\ h_{\{m_j, \dots, m_l\}}^j & \text{if } i = m_j \text{ for some } j \neq l, \\ h_{\{i, m_2, \dots, m_l\}}^1 & \text{if } i \in cl(m_1), \\ x_i - x_{\max cl(i)} & \text{otherwise.} \end{cases}$$

We call the set  $\{\tilde{g}_1, \dots, \tilde{g}_n\}$  a *reduced  $\nu$ -basis*.

*Remark 1.10.* When  $l = k$ , the ideals generated by the polynomials in (1.1) and in (1.2) are the same. This follows because for  $i \in cl(m_1) \setminus \{m_1\}$ , we have  $\tilde{g}_i - \tilde{g}_{m_1} = x_i - x_{m_1} = g_i$ .

**Theorem 1.11.** *A graph  $G$  with  $n$  vertices is uniquely  $k$ -colorable if and only if the reduced Gröbner basis for  $I_{G,k}$  with respect to any term order with  $x_n \prec \dots \prec x_1$  has the form  $\{\tilde{g}_1, \dots, \tilde{g}_n\}$  for polynomials as in (1.2).*

*Remark 1.12.* It is not difficult to test whether a Gröbner basis is of the form given by (1.2). Moreover, the unique coloring can be easily recovered from the reduced Gröbner basis.

In Section 6, we shall discuss the tractability of our algorithms. We hope that they might be used to perform experiments for raising and settling problems in the theory of (unique) colorability.

*Example 1.13.* We present an example of a uniquely 3-colorable graph on  $n = 12$  vertices and give the polynomials  $\tilde{g}_1, \dots, \tilde{g}_n$  from Theorem 1.11.

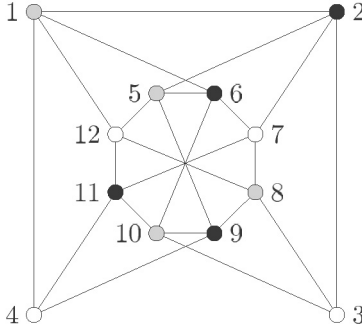


FIGURE 1. A uniquely 3-colorable graph [5].

Let  $G$  be the graph given in Figure 1. The indicated 3-coloring partitions  $V$  into  $k = l = 3$  color classes with  $(m_1, m_2, m_3) = (10, 11, 12)$ . The following set of

12 polynomials is the reduced Gröbner basis for the ideal  $I_{G,k}$  with respect to any term ordering with  $x_{12} \prec \cdots \prec x_1$ . The leading terms of each  $\tilde{g}_i$  are underlined.

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

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

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 Sections 4 and 5, we present proofs for Theorems 1.7, 1.9, and 1.11. Theorems 1.1 and 1.9 give algorithms for testing  $k$ -colorability and unique  $k$ -colorability of graphs, and we discuss the implementation of them in Section 6, along with a verification of a counterexample found by Akbari, Mirrokni, and Sadjad [2] to a conjecture [5, 8, 14] by Xu concerning uniquely 3-colorable graphs without triangles.

## 2. ALGEBRAIC PRELIMINARIES

We briefly review the basic concepts of commutative algebra that will be useful for us here. We refer to [6] or [7] for more details. 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 said to be of *Krull dimension zero* (or simply *zero-dimensional*) if  $V(I)$  is finite. A *term order*  $\prec$  for the monomials of  $R$  is a well-ordering which is multiplicative ( $u \prec v \Rightarrow wu \prec wv$  for monomials  $u, v, w$ ) 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 (i.e.,  $I = \sqrt{I}$ ).
- (2)  $I$  contains a univariate square-free polynomial in each indeterminate.
- (3)  $|\mathcal{B}_{\prec}(I)| = |V(I)|$ .

*Proof.* See [7, p. 229, Proposition 4] and [6, pp. 39–41, Proposition 2.7 and Theorem 2.10].  $\square$

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

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

is generated by the initial terms of elements of  $\mathcal{G}$ . It is called *minimal* if no leading term of  $f \in G$  divides any other leading term of polynomials in  $G$ . Furthermore, a *universal Gröbner basis* is a set of polynomials which is a Gröbner basis with respect to all term orders. 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

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

corresponds to a set difference [7, p. 193, Corollary 8].

### 3. VERTEX COLORABILITY

In what follows, the set of colors  $C_k$  will be the set of  $k$ th roots of unity, and we shall freely speak of points in  $\mathbb{k}^n$  with all coordinates in  $C_k$  as colorings of  $G$ . In this case, a point  $(v_1, \dots, v_n) \in \mathbb{k}^n$  corresponds to a coloring of vertex  $i$  with color  $v_i$  for  $i = 1, \dots, n$ . 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  $\mathbf{v} = (v_1, \dots, v_n) \in V(I_{G,k})$ ; 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  $\mathbf{v} \in V(I_{G,k})$ . If  $\mathbf{v}$  is an improper coloring, then it is easy to see that  $f_G(\mathbf{v}) = 0$ . 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.  $\square$

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).  $\square$

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

**Lemma 3.4.** *Let  $\chi_G$  be the chromatic polynomial of  $G$ . Then*

$$\begin{aligned}\chi_G(k) &= \dim_{\mathbb{k}} R/I_{G,k}, \\ k^n - \chi_G(k) &= \dim_{\mathbb{k}} R/(I_{n,k} + \langle f_G \rangle).\end{aligned}$$

*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  $f(v_1, \dots, v_n) = 0$  for any  $(v_1, \dots, v_n) \in \mathbb{k}^n$  with at most  $k$  of the  $v_i$  distinct. Clearly,  $J_{n,k} \subseteq K_{n,k}$ . We will need the following result of Kleitman and Lovász [12].

**Theorem 3.5** (Kleitman-Lovász). *The ideals  $K_{n,k}$  and  $J_{n,k}$  are the same.*

We now prove Theorem 1.1. We feel that it is the most efficient proof of this result.

*Proof of Theorem 1.1.* (1)  $\Rightarrow$  (2)  $\Rightarrow$  (3): 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  $1 \in I_{G,k}$ .

(3)  $\Rightarrow$  (4): 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  $f_G \in I_{n,k}$ .

(4)  $\Rightarrow$  (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.

(5)  $\Rightarrow$  (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)  $\Rightarrow$  (5): 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. COLORING IDEALS

In this section, we study the  $k$ -coloring ideals  $A_\nu$  mentioned in the introduction and prove Theorem 1.7. Let  $G$  be a graph with proper coloring  $\nu$ , and let  $l \leq k$  be the number of distinct colors in  $\nu(V)$ . For each vertex  $i \in V$ , we assign polynomials  $g_i$  and  $\tilde{g}_i$  as in equations (1.1) and (1.2). 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, to subsets of vertices in different color classes; and the third, to the fact that elements in the same color class should have the same color. These polynomials encode the coloring  $\nu$  algebraically in a computationally useful way (see Lemmas 4.1 and 4.4 below). We begin by showing that the polynomials  $g_i$  are a special generating set for the coloring ideal  $A_\nu$ .

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 any term order with  $x_n \prec \cdots \prec x_1$ . Then the set of polynomials  $\{g_1, \dots, g_n\}$  is a minimal Gröbner basis with respect to  $\prec$  for the ideal  $A_\nu = \langle g_1, \dots, g_n \rangle$  it generates. Moreover, for this ordering, the set  $\{\tilde{g}_1, \dots, \tilde{g}_n\}$  is a reduced Gröbner basis for  $\langle \tilde{g}_1, \dots, \tilde{g}_n \rangle$ .*

*Proof.* Since the initial term of each  $g_i$  (resp.  $\tilde{g}_i$ ) is a power of  $x_i$ , each pair of leading terms is relatively prime. It follows that these polynomials form a Gröbner basis for the ideal they generate. By inspection, it is easy to see that the set of polynomials given by (1.1) (resp. (1.2)) is minimal (resp. reduced).  $\square$

The following innocuous-looking fact is a very important ingredient in the proof of Lemma 4.4.

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

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

for all nonnegative integers  $d$ .

*Proof.* The first step is to note that the polynomial

$$x_i h_U^d + h_{U \setminus \{i\}}^{d+1}$$

is symmetric in the indeterminants  $\{x_\ell : \ell \in U\}$ . This follows from the polynomial identity

$$h_U^{d+1} - h_{U \setminus \{i\}}^{d+1} = x_i h_U^d,$$

and the fact that  $h_U^{d+1}$  is symmetric in the indeterminants  $\{x_\ell : \ell \in U\}$ . Let  $\sigma$  be the permutation  $(i j)$ , and notice that

$$x_i h_U^d + h_{U \setminus \{i\}}^{d+1} = \sigma \left( x_i h_U^d + h_{U \setminus \{i\}}^{d+1} \right) = x_j h_U^d + h_{U \setminus \{j\}}^{d+1}.$$

This completes the proof.  $\square$

We shall also need the following fact that gives explicit representations of some of the generators of  $I_{n,k}$  in terms of those of  $A_\nu$ .

**Lemma 4.3.** *For each  $i = 1, \dots, l$ , we have*

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

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

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

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

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

which is easily seen to cancel the first summand in the sum found in (4.3).

Now, equation (4.3) with  $s = l - i$  gives us that the right hand side of (4.2) is

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

proving the claim (recall that  $m_l = n$ ).  $\square$

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

**Lemma 4.4.** *Let  $g_1, \dots, g_n$  be given as in (1.1). Then the following three properties hold for the ideal  $A_\nu = \langle g_1, \dots, g_n \rangle$ :*

- (1)  $I_{G,k} \subseteq A_\nu$ ,
- (2)  $A_\nu$  is radical,
- (3)  $|V(A_\nu)| = \prod_{j=1}^l (k - l + j)$ .

*Proof.* First assume that  $I_{G,k} \subseteq A_\nu$ . Then  $A_\nu$  is radical from Lemma 2.1, and the number of standard monomials of  $A_\nu$  (with respect to any ordering  $\prec$  as in Lemma 4.1) is equal to  $|V(A_\nu)|$ . Since  $\{g_1, \dots, g_n\}$  is a Gröbner basis for  $A_\nu$  and the initial ideal is generated by the monomials

$$\{x_{m_1}^{k-l+1}, x_{m_2}^{k-l+2}, \dots, x_{m_l}^k\} \text{ and } \{x_i : i \neq m_j \text{ for any } j\},$$

it follows that  $|\mathcal{B}_\prec(A_\nu)| = \prod_{j=1}^l (k - l + j)$ . This proves (3).

We now prove statement (1). From Lemma 4.3, it follows that  $x_i^k - 1 \in A$  when  $i \in \{m_1, \dots, m_l\}$ . It remains to show that  $x_i^k - 1 \in A_\nu$  for all vertices not in  $\{m_1, \dots, m_l\}$ . Let  $f_i = x_i - x_{\max cl(i)}$  and notice that

$$x_{\max cl(i)}^k - 1 = (x_i - f_i)^k - 1 = x_i^k - 1 + f_i h \in A_\nu$$

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

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

$$(4.4) \quad U \subseteq \{m_1, \dots, m_l\} \text{ with } |U| \geq 2 \implies h_U^{k+1-|U|} \in A_\nu.$$

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

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

By induction, the left hand side of this equation is in  $A_\nu$  and therefore the assumption on  $U$  implies that

$$h_{\{v\} \cup U \setminus \{u\}}^{k-s+1} \in A_\nu.$$

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

A similar trick as before using polynomials  $x_i - x_{\max cl(i)} \in A_\nu$  proves that we may replace in (4.4) the requirement that  $U \subseteq \{m_1, \dots, m_l\}$  with one that says that  $U$  consists of vertices in different color classes. Finally, 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  $A_\nu$ . This finishes the proof of the lemma.  $\square$

*Remark 4.5.* Property (1) in the lemma says that  $V(A_\nu)$  contains only proper colorings of  $G$  while properties (2) and (3) say that, up to relabeling the colors, the zeroes of the polynomials  $g_1, \dots, g_n$  correspond to the single proper coloring given by  $\nu$ . The lemma also implies that the polynomials  $\{g_1, \dots, g_n\}$  form a complete intersection.

The decomposition theorem for  $I_{G,k}$  mentioned in the introduction now follows easily from the results of this section.

*Proof of Theorem 1.7.* By Lemmas 3.1 and 4.4, we have

$$V(I_{G,k}) = \bigcup_{\nu} V(A_\nu),$$

where  $\nu$  runs over all proper  $k$ -colorings of  $G$ . Since the ideals  $I_{G,k}$  and  $A_\nu$  are radical by Lemmas 3.2 and 4.4, it follows that:

$$\begin{aligned} I_{G,k} &= I(V(I_{G,k})) \\ &= I\bigcup_{\nu} V(A_\nu) \\ &= \bigcap_{\nu} I(V(A_\nu)) \\ &= \bigcap_{\nu} A_\nu. \end{aligned}$$

This completes the proof.  $\square$

## 5. UNIQUE VERTEX COLORABILITY

We are now in a position to prove our characterizations of uniquely  $k$ -colorable graphs.

*Proof of Theorem 1.9.* (1)  $\Rightarrow$  (2)  $\Rightarrow$  (3): Suppose the graph  $G$  is uniquely  $k$ -colorable and construct the set of  $g_i$  from (1.1) using the proper  $k$ -coloring  $\nu$ . By Theorem 1.7, it follows that  $I_{G,k} = A_\nu$ , and thus the  $g_i$  generate  $I_{G,k}$ .

(3)  $\Rightarrow$  (4): Suppose that  $A_\nu = \langle g_1, \dots, g_n \rangle \subseteq I_{G,k}$ . From Lemma 3.3, we have

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

This proves that  $f_G \in I_{n,k} : \langle g_1, \dots, g_n \rangle$ .

(4)  $\Rightarrow$  (5)  $\Rightarrow$  (1): Assume that  $f_G \in I_{n,k} : \langle g_1, \dots, g_n \rangle$ . Then,

$$I_{n,k} : I_{G,k} = I_{n,k} + \langle f_G \rangle \subseteq I_{n,k} : \langle g_1, \dots, g_n \rangle.$$

Applying Lemmas 2.1 and 4.4, we have

$$(5.1) \quad k^n - k! = |V(I_{n,k}) \setminus V(A_\nu)| = |V(I_{n,k} : A_\nu)| \leq |V(I_{n,k} : I_{G,k})| \leq k^n - k!,$$

since the number of improper colorings is at most  $k^n - k!$ . It follows that equality holds throughout (5.1) so that the number of proper colorings is  $k!$ . Therefore, we have  $\dim_{\mathbb{k}} R/I_{G,k} = k!$  from Lemma 3.4 and  $G$  is uniquely  $k$ -colorable.  $\square$

*Proof of Theorem 1.11.* Suppose that the reduced Gröbner basis of  $I_{G,k}$  with respect to a term order with  $x_n < \dots < x_1$  has the form  $\{\tilde{g}_1, \dots, \tilde{g}_n\}$  as in (1.2). Also, let  $\{g_1, \dots, g_n\}$  be the  $\nu$ -basis (1.1) corresponding to the  $k$ -coloring  $\nu$  read off from  $\{\tilde{g}_1, \dots, \tilde{g}_n\}$ . By Remark 1.10, we have  $\langle g_1, \dots, g_n \rangle = \langle \tilde{g}_1, \dots, \tilde{g}_n \rangle$ . It follows that  $G$  is uniquely  $k$ -colorable from (2)  $\Rightarrow$  (1) of Theorem 1.9. For the other implication, by Lemma 4.1, it is enough to show that  $A_\nu = \langle g_1, \dots, g_n \rangle = I_{G,k}$ , which is (1)  $\Rightarrow$  (2) in Theorem 1.9.  $\square$

## 6. ALGORITHMS AND XU'S CONJECTURE

In this section we describe the algorithms implied by Theorems 1.1 and 1.9, and illustrate their usefulness by disproving a conjecture of Xu.<sup>1</sup> We also present some data to illustrate their runtimes under different circumstances.

From Theorem 1.1, we have the following four methods for determining  $k$ -colorability. They take as input a graph  $G$  with vertices  $V = \{1, \dots, n\}$  and edges  $E$ , and a positive integer  $k$ , and output TRUE if  $G$  is  $k$ -colorable and otherwise FALSE.

- 1: **function** ISCOLORABLE( $G, k$ ) [Theorem 1.1 (2)]
- 2:     Compute a Gröbner basis  $\mathcal{G}$  of  $I_{G,k}$ .
- 3:     Compute the vector space dimension of  $R/I_{G,k}$  over  $\mathbb{k}$ .
- 4:     **if**  $\dim_{\mathbb{k}} R/I_{G,k} = 0$  **then return** FALSE **else return** TRUE.
- 5: **end function**

- 1: **function** ISCOLORABLE( $G, k$ ) [Theorem 1.1 (3)]
- 2:     Compute a Gröbner basis  $\mathcal{G}$  of  $I_{G,k}$ .
- 3:     Compute the normal form  $\text{nf}_{\mathcal{G}}(1)$  of  
          the constant polynomial 1 with respect to  $\mathcal{G}$ .
- 4:     **if**  $\text{nf}_{\mathcal{G}}(1) = 0$  **then return** FALSE **else return** TRUE.
- 5: **end function**

- 1: **function** ISCOLORABLE( $G, k$ ) [Theorem 1.1 (4)]
- 2:     Set  $\mathcal{G} := \{x_i^k - 1 : i \in V\}$ .
- 3:     Compute the normal form  $\text{nf}_{\mathcal{G}}(f_G)$  of  
          the graph polynomial  $f_G$  with respect to  $\mathcal{G}$ .
- 4:     **if**  $\text{nf}_{\mathcal{G}}(f_G) = 0$  **then return** FALSE **else return** TRUE.
- 5: **end function**

- 1: **function** ISCOLORABLE( $G, k$ ) [Theorem 1.1 (5)]
- 2:     Let  $\mathcal{H}$  be the set of graphs with vertices  $\{1, \dots, n\}$   
          consisting of a clique of size  $k + 1$  and isolated vertices.
- 3:     Set  $\mathcal{G} := \{f_H : H \in \mathcal{H}\}$ .
- 4:     Compute the normal form  $\text{nf}_{\mathcal{G}}(f_G)$  of  
          the graph polynomial  $f_G$  with respect to  $\mathcal{G}$ .

---

<sup>1</sup>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/>.

```

5:   if  $\text{nf}_{\mathcal{G}}(f_G) = 0$  then return FALSE else return TRUE.
6: end function

```

From Theorem 1.9, we have the following three methods for determining unique  $k$ -colorability. They take as input a graph  $G$  with vertices  $V = \{1, \dots, n\}$  and edges  $E$ , and output TRUE if  $G$  is uniquely  $k$ -colorable and otherwise FALSE. Furthermore, the first two methods take as input a proper  $k$ -coloring  $\nu$  of  $G$  that uses all  $k$  colors, while the last method requires a positive integer  $k$ .

```

1: function ISCOLORABLE( $G, \nu$ ) [Theorem 1.9 (3)]
2:   Compute a Gröbner basis  $\mathcal{G}$  of  $I_{G,k}$ .
3:   for  $i \in V$  do
4:     Compute the normal form  $\text{nf}_{\mathcal{G}}(g_i)$  of
       the polynomial  $g_i$  with respect to  $\mathcal{G}$ .
5:     if  $\text{nf}_{\mathcal{G}}(g_i) \neq 0$  then return FALSE.
6:   end for
7:   return TRUE.
8: end function

```

```

1: function ISCOLORABLE( $G, \nu$ ) [Theorem 1.9 (4)]
2:   Compute a Gröbner basis  $\mathcal{G}$  of  $I_{n,k} : \langle g_1, \dots, g_n \rangle$ .
3:   Compute the normal form  $\text{nf}_{\mathcal{G}}(f_G)$  of
       the graph polynomial  $f_G$  with respect to  $\mathcal{G}$ .
4:   if  $\text{nf}_{\mathcal{G}}(f_G) = 0$  then return TRUE else return FALSE.
5: end function

```

```

1: function ISCOLORABLE( $G, k$ ) [Theorem 1.9 (5)]
2:   Compute a Gröbner basis  $\mathcal{G}$  of  $I_{G,k}$ .
3:   Compute the vector space dimension of  $R/I_{G,k}$  over  $\mathbb{k}$ .
4:   if  $\dim_{\mathbb{k}} R/I_{G,k} = k!$  then return TRUE else return FALSE.
5: end function

```

*Remark 6.1.* It is possible to speed up the above algorithms dramatically by doing some of the computations iteratively. First of all, step 2 of methods (2) and (3) of Theorem 1.1, and methods (3) and (5) of Theorem 1.9 should be replaced by the following code

```

1: Set  $I := I_{n,k}$ .
2: for  $\{i, j\} \in E$  do
3:   Compute a Gröbner basis  $\mathcal{G}$  of  $I + \langle x_i^{k-1} + x_i^{k-2}x_j + \dots + x_i x_j^{k-2} + x_j^{k-1} \rangle$ .
4:   Set  $I := \langle \mathcal{G} \rangle$ .
5: end for

```

Secondly, the number of terms in the graph polynomial  $f_G$  when fully expanded may be very large. The computation of the normal form  $\text{nf}_{\mathcal{G}}(f_G)$  of the graph polynomial  $f_G$  in methods (4) and (5) of Theorem 1.1, and method (4) of Theorem 1.9 should therefore be replaced by the following code

- 1: Set  $f := 1$ .
- 2: **for**  $\{i, j\} \in E$  with  $i < j$  **do**
- 3:     Compute the normal form  $\text{nf}_{\mathcal{G}}((x_i - x_j)f)$  of  $(x_i - x_j)f$  with respect to  $\mathcal{G}$ , and set  $f := \text{nf}_{\mathcal{G}}((x_i - x_j)f)$ .
- 4: **end for**

In [14], Xu showed that if  $G$  is a uniquely  $k$ -colorable graph with  $|V| = n$  and  $|E| = m$ , then  $m \geq (k-1)n - \binom{k}{2}$ , and this bound is best possible. He went on to conjecture that if  $G$  is uniquely  $k$ -colorable with  $|V| = n$  and  $|E| = (k-1)n - \binom{k}{2}$ , 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 ad hoc (although their proof generalizes readily to show that an infinite family of graphs contradicts Xu's conjecture). We verified that this graph is indeed a counterexample to Xu's conjecture using several of the above mentioned methods. The fastest verification requires less than two seconds of processor time on a laptop PC with a 1.5 GHz Intel Pentium M processor and 1.5 GB of memory. The code can be downloaded from the link at the beginning of this section. The speed of these calculations should make the testing of conjectures for uniquely colorable graphs a more tractable enterprise.

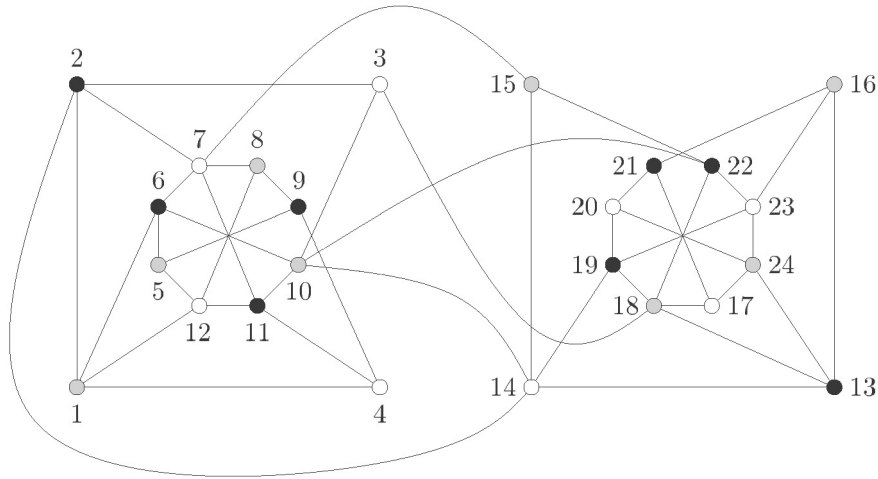


FIGURE 2. A counterexample to Xu's conjecture [2].

Below are the runtimes for the graphs in Figures 1 and 2. The term orders used are given in the notation of the computational algebra program Singular: lp is the lexicographical ordering, Dp is the degree lexicographical ordering, and dp is the degree reverse lexicographical ordering. That the computation did not finish within 10 minutes is denoted by "> 600", while "-" means that the computation ran out of memory.

Characteristic	0			2		
	lp	Dp	dp	lp	Dp	dp
Theorem 1.1 (2)	3.28	2.29	1.24	2.02	1.56	0.81
Theorem 1.1 (3)	3.30	2.42	1.25	2.15	1.60	0.94
Theorem 1.1 (4)	1.86	> 600	> 600	1.08	448.28	324.89
Theorem 1.1 (5)	> 600	> 600	> 600	> 600	> 600	> 600
Theorem 1.9 (3)	3.53	2.54	1.43	2.23	1.72	1.03
Theorem 1.9 (4)	> 600	> 600	> 600	> 600	> 600	> 600
Theorem 1.9 (5)	3.30	2.28	1.24	2.03	1.54	0.82

Runtimes in seconds for the graph in Figure 1.

Characteristic	0			2		
	lp	Dp	dp	lp	Dp	dp
Theorem 1.1 (2)	596.89	33.32	2.91	144.05	12.45	1.64
Theorem 1.1 (3)	598.25	33.47	2.87	144.60	12.44	1.81
Theorem 1.1 (4)	–	> 600	> 600	–	> 600	> 600
Theorem 1.1 (5)	> 600	> 600	> 600	> 600	> 600	> 600
Theorem 1.9 (3)	597.44	34.89	4.29	145.81	13.55	3.02
Theorem 1.9 (4)	–	–	–	–	–	–
Theorem 1.9 (5)	595.97	33.46	2.94	145.02	12.34	1.64

Runtimes in seconds for the graph in Figure 2.

Another way one can prove that a graph is uniquely  $k$ -colorable is by computing the chromatic polynomial and testing if it equals  $k!$  when evaluated at  $k$ . This is possible for the graph in Figure 1. Maple reports that it has chromatic polynomial

$$x(x-2)(x-1)(x^9 - 20x^8 + 191x^7 - 1145x^6 + 4742x^5 - 14028x^4 + 29523x^3 - 42427x^2 + 37591x - 15563).$$

When evaluated at  $x = 3$  we get the expected result  $6 = 3!$ . Computing the above chromatic polynomial took 94.83 seconds. Maple, on the other hand, was not able to compute the chromatic polynomial of the graph in Figure 2 within 10 hours.

## 7. ACKNOWLEDGMENTS

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