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## ALGEBRAIC AND COMBINATORIAL PROPERTIES OF CERTAIN TORIC IDEALS IN THEORY AND APPLICATIONS

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ABSTRACT OF DISSERTATION

Sonja Petrović

The Graduate School  
University of Kentucky

2008

ALGEBRAIC AND COMBINATORIAL PROPERTIES OF CERTAIN TORIC  
IDEALS IN THEORY AND APPLICATIONS

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ABSTRACT OF DISSERTATION

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A dissertation submitted in partial fulfillment of the  
requirements of the degree of Doctor of Philosophy in the  
College of Arts and Sciences at the University of Kentucky

By

Sonja Petrović

Lexington, Kentucky

Director: Dr. Uwe Nagel, Department of Mathematics

Lexington, Kentucky

2008

## ABSTRACT OF DISSERTATION

### ALGEBRAIC AND COMBINATORIAL PROPERTIES OF CERTAIN TORIC IDEALS IN THEORY AND APPLICATIONS

This work focuses on commutative algebra, its combinatorial and computational aspects, and its interactions with statistics. The main objects of interest are projective varieties in  $\mathbb{P}^n$ , algebraic properties of their coordinate rings, and the combinatorial invariants, such as Hilbert series and Gröbner fans, of their defining ideals. Specifically, the ideals in this work are all toric ideals, and they come in three flavors: they are defining ideals of a family of classical varieties called rational normal scrolls, cut ideals that can be associated to a graph, and phylogenetic ideals arising in a new and increasingly popular area of algebraic statistics.

Sonja Petrović

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May 2008

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ALGEBRAIC AND COMBINATORIAL PROPERTIES OF CERTAIN TORIC  
IDEALS IN THEORY AND APPLICATIONS

By  
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May 2008

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(Date)



DISSERTATION

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## ACKNOWLEDGMENT

”The two operations of our understanding, intuition and deduction, on which alone we have said we must rely in the acquisition of knowledge.”

–Rene Descartes

This work has benefited greatly from the teachings and insights of my adviser, Uwe Nagel. I am deeply grateful for his endless support, dedication, and motivation to pursue the research program described in this dissertation. He has instilled in me a curiosity which does not end with this work. In addition, I am indebted to Alberto Corso for his continuous guidance and support during the past few years. I would also like to thank the rest of the Dissertation Committee, Arne Bathke, David Leep, and the outside examiner, Kert Viele, for the time they have spent on this dissertation and its defense.

The five years I spent at the University of Kentucky would not have been so delightful without my dear friend and collaborator, Julia Chifman, with whom I have shared research projects, teaching problems, office space, and many mathematical ideas. There are many more people to whom I am grateful for motivating discussions, of which I must single out Bernd Sturmfels, Seth Sullivant, and Ruriko Yoshida.

I would not be where I am today without the love and support of my family, relatives, and friends. I owe everything to Mama, Tata and Bojan, for it is their sacrifice and positive energy during the hardest of times that have made my education possible. They have inspired me to take every opportunity that knocks on my door. And last, but not least, I am most grateful to Saša for always being there to pick me up when I fall, for helping me believe in myself, and for teaching me that no matter what happens today, we should never lose hope for a better tomorrow.

As a wise man once said, the world is round and the place which may seem like the end may also be only the beginning.

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file size: 479KB

## Chapter 1

### Introduction

Commutative algebra, its combinatorial and computational aspects, and its interactions with statistics and applications to biology, have received quite a lot of attention recently, as pointed out in a recent issue of SIAM News ([43]). The foundational work of many authors established a thrilling connection between algebra, statistics and computational biology. Toric ideals and their combinatorial invariants, such as Hilbert series and Gröbner fans, play an essential role in the area. Additionally, the applied problems motivate a deeper study of both classical and new ideals from a purely algebraic point of view.

Inspired by the works of Allman, Rhodes, Sullivant, Sturmfels and their collaborators, we embark on a study of toric ideals of some well-known varieties called rational normal scrolls, toric ideals that record algebraic relations among the cuts of a graph, and toric ideals arising in phylogenetics, a new area in algebraic statistics focusing on computational biology.

Some of the projects described here are inspired by the interplay of the pure and the applied, while others seek a generalization of some well-known results that admit a combinatorial approach. The thread connecting them is the theory of Gröbner bases and their special structure in the case of toric ideals.

#### 1.1 Universal Gröbner bases of rational normal scrolls

Gröbner bases are the foundation of most computations involving polynomials. In addition, their special structure may provide powerful theoretical consequences. Given a term order, any generating set of an ideal  $I$  can be transformed into a (reduced) Gröbner basis ([34]). The *universal Gröbner basis*  $\mathcal{U}_I$  is the union of all of the (finitely many) reduced Gröbner bases of the ideal  $I$ . It is known that  $\mathcal{U}_I$  is contained in the *Graver basis*  $\mathcal{G}_I$ , which is the set of all primitive elements in the ideal. Obtaining an explicit description of either of these sets, or a *sharp* degree bound for their elements, is a nontrivial task.

We propose a solution to this problem for varieties of minimal degree, which are the varieties that attain the general lower bound on the degree. They have been classified as the quadratic hypersurfaces, the Veronese surface in  $\mathbb{P}^5$ , the rational normal scrolls, and the cones over these. Except for quadratic hypersurfaces, all of their defining ideals are toric.

In their '95 paper [21], Graham, Diaconis and Sturmfels give a nice combinatorial description of the Graver basis for any rational normal curve in terms of primitive partition identities. Motivated by a discussion with Bernd Sturmfels, we extend this concept and define a *colored* partition identity. This allows us to generalize the result for curves, which appears in [30]:

**Theorem (3.3.8).** *The elements of the Graver basis of any rational normal scroll are precisely the color-homogeneous primitive colored partition identities.*

From the combinatorial description of the Graver basis elements, we derive a sharp bound on their degrees, and show that, somewhat surprisingly, it is always attained by a two-colored circuit. The set of *circuits*  $\mathcal{C}_I$  is a subset of  $\mathcal{U}_I$  consisting of the primitive elements with minimal support. An important consequence of the Theorem is the following:

**Corollary (3.4.6).** *If  $X$  is a variety that can be obtained from a scroll by a sequence of projections to some of the coordinate hyperplanes, then the degree of  $X$  is an upper bound on the degree of any element in the universal Gröbner basis of its defining ideal.*

The bound also holds for the Graver basis, and it is always better than the general bound for the toric ideals given in [34]. In general, however, it is unknown whether the degree of the variety is an upper bound for even a *single* reduced Gröbner basis. Note that the set of circuits  $\mathcal{C}_I$  is in general properly contained in the universal Gröbner basis  $\mathcal{U}_I$ , which in turn is a proper subset of the Graver basis  $\mathcal{G}_I$ . However, extensive computations show evidence supporting the following:

**Conjecture 1.1.1.** *The universal Gröbner basis and the Graver basis of the ideal of every rational normal scroll agree.*

In general, it is an open problem to characterize those (toric) ideals for which the equalities hold in either of the containments  $\mathcal{C}_I \subset \mathcal{U}_I \subset \mathcal{G}_I$ . There are examples of families of ideals whose circuits equal the Graver basis, for example Sturmfels shows the property for toric ideals defined by unimodular matrices, and Villarreal for those defined by balanced matrices.

## 1.2 Toric ideals of phylogenetic invariants

Most of the material in this section is drawn from a joint paper with J. Chifman [11]. The main problem of the project was to understand and explicitly describe generating sets of a family of toric ideals with an applied flavor: certain ideals of phylogenetic invariants. They arise in studying statistical models of evolution, with the goal of reconstructing ancestral relationship between species. This relationship can be represented using a phylogenetic tree, which is defined to be a directed acyclic simple graph equipped with some statistical information ([2],[29],[35]).

There is a specific class of models, namely group-based models, for which the ideals of invariants are toric. Sturmfels and Sullivant in [35] reduce their computation to the case of claw trees  $K_{1,n}$ , the complete bipartite graph from one node (the root) to  $n$  nodes (the leaves). The main result of [35] gives a way of constructing the ideal of phylogenetic invariants for any tree *if* the ideal for the claw tree is known. However, in general, it is an open problem to compute the phylogenetic invariants for a claw tree. We solve it for the general group-based model when the group is  $\mathbb{Z}_2$ , the smallest group of interest in applications.

**Theorem** (4.5.7, 4.5.9). *For  $n \geq 4$ , the ideal of phylogenetic invariants on a claw tree on  $n$  leaves has a squarefree quadratic lexicographic Gröbner basis. Moreover, these sets of generators can be obtained recursively.*

Combined with the main result of Sturmfels and Sullivant in [35], this implies that the phylogenetic ideal of *every* tree for the group  $\mathbb{Z}_2$  has a quadratic squarefree Gröbner basis that can be explicitly constructed. Hence, the coordinate ring of the toric variety is a Koszul algebra and a Cohen-Macaulay ring.

These ideals are particularly nice as they satisfy the conjecture in [35] which proposes that the order of the group gives an upper bound for the degrees of minimal generators of the ideal of invariants. In general, the conjecture is open.

The phylogenetic ideals of claw trees can be studied as a natural subfamily of a more general class of ideals, which are described next.

### 1.3 Cut ideals of graphs

Let  $G$  be any simple graph. Any unordered partition  $A|B$  of its vertices induces a coloring on the edges of the graph in the following way: label by  $t_e$  an edge  $e$  if it connects two vertices in the same partition, and by  $s_e$  the edges that connect two vertices from the different partitions. This way, any cut gives rise to a monomial in the variables  $s_e, t_e$  as  $e$  ranges over the edge set of  $G$ . The cut ideal of  $G$  records the algebraic relations among the cuts, and defines a projective variety  $X_G$ .

These toric ideals have been introduced by Sturmfels and Sullivant who also proposed relating their properties to the combinatorial structure of the graph. Some of the conjectures posed in [36] are:

- The set of all graphs generated in degree at most  $k$  is minor-closed for any  $k$ , where a minor of  $G$  is a graph obtained from  $G$  by contracting and deleting edges.
- The cut ideal  $I_G$  is generated in degree two if and only if  $G$  is free of  $K_4$  minors, where  $K_4$  is the complete graph on 4 vertices.
- The coordinate ring of the variety  $X_G$  is Cohen-Macaulay if and only if  $G$  is free of  $K_5$  minors, where  $K_5$  is the complete graph on 5 vertices.

Our interest in these problems began with the realization that the cut ideals are a natural generalization of phylogenetic ideals from [11]: the phylogenetic ideal on the claw tree with  $n$  leaves is isomorphic to the cut ideal of an  $(n + 1)$ -cycle. This correspondence immediately provides the following:

**Theorem** (5.3.3). *The cut ideal of a  $k$ -cycle has a quadratic lexicographic Gröbner basis for  $k \geq 4$ . In addition, the Gröbner basis is squarefree. Thus, the cut varieties of cycles are arithmetically Cohen-Macaulay.*

Sometimes one can build a graph by overlapping two smaller graphs on a common complete subgraph, or a clique. If the clique is small enough, Sturmfels and Sullivan give a way of constructing the cut ideal of the big graph from the smaller ones. In a joint paper with Nagel on cut ideals of graphs [28], we use this powerful construction extensively.

**Theorem (5.6.2).** *If a graph can be built from trees and cycles using small clique sums ( $k \leq 2$ ), then its cut ideal has a squarefree quadratic Gröbner basis, thus in particular it is generated in degree two. In addition, the coordinate rings are Cohen-Macaulay and Koszul.*

The theorem implies the quadratic generation conjecture for a large family of graphs free of  $K_4$ -minors. In fact, we can describe deformations of cut ideals in a way that reduces the quadratic generation conjecture to the case of subdivisions of books, which have been treated by Brennan and Chen in [6]. Hence we obtain:

**Theorem (5.6.6).** *The cut ideal  $I_G$  is generated in degree two if and only if  $G$  is free of  $K_4$  minors.*

This thesis is organized as follows: Chapter 2 contains some of the necessary background material. In it we briefly recall main definitions and results from commutative algebra and the theory of Gröbner bases of toric ideals. The subsequent Chapters are devoted to the study of the three classes of toric ideals described in this Introduction: in Chapter 3 we describe universal Gröbner bases of rational normal scrolls. Chapter 4 takes on a more applied flavor, where we obtain Gröbner bases of the ideals of phylogenetic invariants and explore some of their surprising properties. In Chapter 5 we turn the study of ideals which generalize those arising in phylogenetics: cut ideals of graphs. We will see that several important families of graphs have cut ideals with very nice, and perhaps unexpected, algebraic properties.

## Chapter 2

### Background

We recall some facts and terminology about projective varieties, toric ideals, and their Gröbner bases. For a more thorough introduction to these concepts, the reader should refer to the books by Eisenbud [17] and Sturmfels [34].

#### 2.1 Ideals and Varieties

Unless otherwise stated,  $S$  will denote the polynomial ring  $K[x_0, \dots, x_n]$  in  $n + 1$  variables over the field  $K$ . (We usually assume  $K = \mathbb{C}$  for applications.)

Let  $V$  be a vector space over the field  $K$ . Then the *projective space*  $\mathbb{P}(V)$  is the set of 1-dimensional subspaces of  $V$ . A *point* of  $\mathbb{P}(V)$  is just a 1-dimensional subspace (a line through the origin). The *dimension* of  $\mathbb{P}(V)$  is  $\dim(V) - 1$ . If  $V = K^{n+1}$ , then we set  $\mathbb{P}^n := \mathbb{P}_k^n := \mathbb{P}(K^{n+1})$ . We say a point  $P \in \mathbb{P}^n$  has *coordinates*  $(x_0 : \dots : x_n)$  if  $P$  is the line spanned by the  $(n + 1)$ -tuple  $0 \neq (x_0, \dots, x_n) \in K^{n+1}$ .

A *projective variety* is a subset of  $\mathbb{P}^n$  that is the locus of common zeros of *homogeneous* polynomials  $(f_\lambda)_{\lambda \in \Lambda}$ , where  $f_\lambda \in K[x_0, \dots, x_n]$ . Recall that a polynomial is called *homogeneous* (with respect to the standard grading  $\deg(x_i) = 1$ ) if all of its monomials have the same degree.

**Definition 2.1.1.** (a) Let  $I \subset S$  be a homogeneous ideal. Then

$$V(I) := \{P \in \mathbb{P}^n : f(P) = 0 \text{ for all } f \in I\}$$

is the *projective variety* defined by  $I$ .

(b) If  $X \subset \mathbb{P}^n$  is any subset, then  $I(X)$  is the ideal generated by all homogeneous polynomials  $f \in S$  such that  $f$  vanishes on all of  $X$ .

(c) If  $X \subset \mathbb{P}^n$  is a projective variety, then  $A_X := S/I(X)$  is called the *homogeneous coordinate ring of  $X$* . It is a graded ring.

To illustrate the definition, we provide a family of examples which will be used in the following chapter.

**Example 2.1.2.** [Rational normal curve] Consider the parametrization map

$$\begin{aligned} \varphi : S &\rightarrow [s^n, s^{n-1}t, \dots, st^{n-1}, t^n] =: R \\ x_i &\mapsto s^i t^{n-i}. \end{aligned}$$

Then  $\ker \varphi = I_C$  the ideal of the rational normal curve in  $\mathbb{P}^n$ . It is a homogeneous ideal, as it can be shown that it is generated by 2-minors of a certain matrix of indeterminants. The 2-minors are homogeneous binomials of degree 2.



In general, for a homogeneous ideal  $a \subset m$  where  $m := (x_0, \dots, x_n)$ , denote by  $a^{sat}$  the *saturation* of  $a$  obtained by essentially removing  $m$  from the set of associated primes of  $a$ .

**Definition 2.1.3.** Let  $a \subset m$  be a homogeneous ideal. We consider  $S/a^{sat}$  as a geometric object called the *projective scheme*  $X \subset \mathbb{P}^n$  defined by  $a$ . The homogeneous ideal of  $X$  is  $I_X := a^{sat}$ , and the *homogeneous coordinate ring* of  $X$  is  $A_X := S/a^{sat}$ .

In addition, recall that a *graded  $S$ -module* is an  $S$ -module  $M$  that admits a decomposition as a direct sum (as  $K$ -modules) of graded components:

$$M = \bigoplus_{j \geq 0} [M]_j$$

such that  $[S]_i \cdot [M]_j \subset [M]_{i+j}$ .

The elements in  $[M]_j$  are called *homogeneous of degree  $j$* .

Next we would like to define some invariants that capture the algebraic information about  $I$ . We define a Hilbert function of a variety, which essentially counts the number of monomials of each degree not appearing in the defining ideal of the variety.

**Definition 2.1.4.** (a) Let  $M$  be a finitely generated graded  $S$ -module. Then its *Hilbert function* in degree  $j$  is the vector space dimension of its  $j^{th}$  graded component:

$$\begin{aligned} h_M : \mathbb{Z} &\rightarrow \mathbb{Z} \\ h_M(j) &= \dim_K [M]_j \end{aligned}$$

(b) The *Hilbert function* of the projective subscheme  $X \subset \mathbb{P}^n$  is the Hilbert function of its coordinate ring:

$$h_X := h_{S/I_X}.$$

Note that  $h_X(j)$  measures the number of hypersurfaces of degree  $j$  (that is, varieties defined by polynomials of degree  $j$ ) that do not contain  $X$ .

**Example 2.1.5.** 1. The Hilbert function in degree  $j$  of the polynomial ring in  $n + 1$  variables is the number of monomials of degree  $j$ :

$$h_S(j) = \begin{cases} \binom{n+j}{n} & \text{for } j \geq 0 \\ 0 & \text{if } j < 0. \end{cases}$$

2. (Example 2.1.2, continued) Consider the ideal of the rational normal curve  $I_C$ . Since  $I_C = \ker \varphi$  for  $\varphi([S]_j) = [R]_{nj}$ ,

$$h_C(j) = h_{R/I_C}(j) = \dim_k \varphi([S]_j) = \dim [K[s, t]]_{nj} = \begin{cases} nj + 1 & \text{if } j \geq 0 \\ 0 & \text{if } j < 0. \end{cases}$$

In addition, one might ask what the dimension and degree of a variety are. These notions should generalize the intuitive notions of dimension and degree.

**Theorem 2.1.6 (and Definition).** *Let  $M$  be a finitely generated  $S$ -module. Then there exists a polynomial  $p_M \in \mathbb{Q}[t]$  such that  $h_M(j) = p_M(j)$  for all  $j \gg 0$ . The polynomial  $p_M$  is called the Hilbert polynomial of  $M$ . It can be written as*

$$p_M(t) = h_0(M) \binom{t+d}{d} + h_1(M) \binom{t+d-1}{d-1} + \cdots + h_d(M),$$

where  $h_0(M), \dots, h_d(M) \in \mathbb{Z}$ . The degree of  $M$  is

$$\deg M = \begin{cases} h_0(M) & \text{if } p_M \neq 0 \\ \dim_K M & \text{if } p_M = 0. \end{cases}$$

If  $M \neq 0$ , then  $\deg M > 0$ . The (Krull) dimension of  $M$  is

$$\dim M = \begin{cases} 1 + \deg p_M & \text{if } p_M \neq 0 \\ 0 & \text{if } p_M = 0. \end{cases}$$

For a subscheme  $X \in \mathbb{P}^n$ , with coordinate ring  $A_X := S/I_X$ , the degree is defined as  $\deg X := \deg A_X$  and  $\dim X = \dim A_X - 1 = \deg p_X$ , with  $p_X := p_{A_X}$ .

Note that the degree of  $X$  is the *multiplicity* of the coordinate ring  $A_X$ . Let us illustrate these definitions with some examples:

**Example 2.1.7.** 1. From the previous example, we know the Hilbert function and thus the Hilbert polynomial of the polynomial ring in  $n+1$  variables:

$$p_{\mathbb{P}^n}(t) = \binom{n+t}{n} = \frac{(n+t) \cdots (t+1)}{n!},$$

thus  $\deg \mathbb{P}^n = 1$  and  $\dim \mathbb{P}^n = n$ .

2. If  $X$  is a hypersurface defined by  $I_X = (f)$  with  $f \in [S]_d$ , then

$$p_X = \binom{n+t}{n} - \binom{n+t-d}{n},$$

thus  $\dim X = n - 1$  and  $\deg X = d$ .

3. Let  $C$  be a rational normal curve in  $\mathbb{P}^n$ . Then we have already seen that  $p_C(t) = nt + 1$ , hence  $\dim C = 1$  (thus justifying the name "curve") and  $\deg C = n$ .

**Definition 2.1.8.** The *Hilbert series* of a variety  $X \subset \mathbb{P}^n$  is the formal power series

$$H_X(t) = \sum_{i \geq 0} h_{A_X}(i) t^i.$$

It is a rational function that can be uniquely written as

$$H_X(t) = \frac{h_0 + h_1 t + \cdots + h_s t^s}{(1-t)^d},$$

where  $d$  is the (Krull) dimension of  $A_X$ ,  $h_0 = 1, h_1, \dots, h_s$  are integers, and  $h_s \neq 0$ . If  $A_X$  is Cohen-Macaulay, then all  $h_i$  are non-negative and  $(h_0, \dots, h_s)$  is called the *h-vector* of  $A_X$ .

$X$  comes with one more invariant of interest, the regularity.

**Definition 2.1.9.** Consider a *minimal free resolution* of  $M$ :

$$0 \rightarrow F_s \rightarrow \cdots \rightarrow F_0 \rightarrow M \rightarrow 0$$

with  $F_i := \bigoplus_j S(-a_{ij})$ . Then the *Castelnuovo-Mumford regularity* of  $M$ , denoted by  $\text{reg}(M)$ , is defined as:

$$\text{reg}(M) := \max\{a_{ij} - i : i, j \in \mathbb{Z}\}.$$

The Castelnuovo-Mumford regularity of a variety  $X \subset \mathbb{P}^n$  is defined as  $\text{reg } X := \text{reg } A_X + 1$ .

Here is another set of examples for which dimension and degree are not hard to compute.

**Definition 2.1.10.**  $X \in \mathbb{P}^n$  is called a *complete intersection* of type  $(d_1, \dots, d_c)$  if  $I_X = (f_1, \dots, f_c)$  where  $\deg f_i = d_i$ , and  $f_1, \dots, f_c$  is a *regular sequence*; i.e.  $f_i$  is not a zero divisor in  $S/(f_1, \dots, f_{i-1})S$  for each  $i$ .

In case of a complete intersection, it is easy to calculate the dimension and degree:  $\dim X = n - c$  and  $\deg X = d_1 \dots d_c$ . Let us also introduce another class of special varieties to which each complete intersection belongs. For that we need the concept of a *depth* of a module:

**Definition 2.1.11.** Let  $M$  be a finitely generated  $S$ -module. Then the length of *each* maximal  $M$ -regular sequence is called the *depth* of  $M$ ,  $\text{depth}(M)$ .

In general, the bound  $\text{depth}(M) \leq \dim(M)$  holds. The special varieties we are interested in are those that achieve equality:

**Definition 2.1.12.** (a)  $M$  is called a *Cohen-Macaulay* module (*CM*) if  $\text{depth}(M) = \dim(M)$ .

(b) A ring  $R$  is a Cohen-Macaulay ring if it is Cohen-Macaulay as an  $R$ -module.

(c) If  $X \subset \mathbb{P}^n$  is a subscheme, then  $X$  is said to be *arithmetically Cohen-Macaulay* (*aCM*) if the coordinate ring  $S/I_X$  is a CM ring.

We will see in Section 2.2 how special structure of Gröbner bases of an ideal provides information about the Cohen-Macaulayness of its coordinate ring. Another property of the coordinate ring, Koszulness, will also be implied by a special structure of a Gröbner basis:

**Definition 2.1.13.** The ring  $S/I$  is *Koszul* if the field  $K$  has a linear resolution as a graded  $S/I$ -module:

$$\cdots \rightarrow (S/I)^{\beta_2}(-2) \rightarrow (S/I)^{\beta_1}(-1) \rightarrow S/I \rightarrow K \rightarrow 0.$$

The implications will be explained in detail in Section 2.2.

## 2.2 Gröbner bases of toric ideals

For convenience of notation, in this section the polynomial ring  $S$  will have  $n$  variables:

$$S := k[x_1, \dots, x_n].$$

A total order  $\prec$  on the monomials of  $S$  is called a *term order* if 0 is the unique minimal element, and if  $m_1 \prec m_2$  implies  $mm_1 \prec mm_2$ , where  $m, m_1$  and  $m_2$  are any monomials.

**Example 2.2.1.** The (*degree*) *lexicographic* term order induced by  $x_1 > x_2 > \cdots > x_n$  is defined as follows:

$$m_1 \prec_{lex} m_2$$

if either  $\deg(m_1) < \deg(m_2)$  or  $\deg(m_1) = \deg(m_2)$  and the smallest index of a variable appearing in  $m_1$  is bigger than the smallest index of a variable appearing in  $m_2$ . For example,  $x_1^2 x_2 x_3 \succ_{lex} x_2^4$  due to the appearance of  $x_1$ .

Another frequently used term order is the *degree reverse lexicographic order*:

$$m_1 \prec_{revlex} m_2$$

if either  $\deg(m_1) < \deg(m_2)$  or  $\deg(m_1) = \deg(m_2)$  and the largest index of a variable appearing in  $m_1$  is smaller than the largest index of a variable appearing in  $m_2$ . For example,  $x_1^2 x_2 x_3 \prec_{revlex} x_2^4$ , due to the appearance of  $x_3$ .

Given a term order, every non-zero polynomial  $f \in S$  has a unique *initial term*, denoted by  $in_{\prec}(f)$ .

**Definition 2.2.2.** The initial ideal of  $I \subset S$  with respect to the term order  $\prec$  is defined to be the following monomial ideal:  $in_{\prec}(I) := (in_{\prec}(f) : f \in I)$ . Any generating set  $\mathcal{G}_{\prec}$  of the ideal such that  $in_{\prec}(I) = (in_{\prec}(g) : g \in \mathcal{G}_{\prec})$  is called a *Gröbner basis*.

The Gröbner basis  $\mathcal{G}_{\prec}$  is called *reduced* if for each  $g \in \mathcal{G}_{\prec}$ , no term of  $g$  is divisible by  $in_{\prec}(f)$  for any other Gröbner basis element  $f \in \mathcal{G}_{\prec}$ . For any ideal  $I$ , the reduced Gröbner basis  $\mathcal{G}_{\prec}$  is uniquely determined by the term order  $\prec$ .

To calculate a Gröbner basis of  $I$ , one can use Buchberger's algorithm. It makes use of the multivariate division algorithm:

**Algorithm 2.2.3** (Division Algorithm). Consider the ideal  $I \subset S$  and a fixed monomial order. If  $f, g_1, \dots, g_t \in I$ , we can produce an expression  $f = \sum m_u g_{s_u} + f'$  for  $f$  with respect to  $g_1, \dots, g_t$  by defining the indices  $s_u$  and the terms  $m_u$  inductively;  $f'$  is called the *remainder* of division of  $f$  by  $g_1, \dots, g_t$ . Having chosen  $s_1, \dots, s_p$  and  $m_1, \dots, m_p$ , if

$$f'_p := f - \sum_{u=1}^p m_u g_{s_u} \neq 0$$

and  $m$  is the maximal term of  $f'_p$  that is divisible by *some*  $\text{in}(g_i)$ , then we choose

$$\begin{aligned} s_{p+1} &= i, \\ m_{p+1} &= m / \text{in}(g_i). \end{aligned}$$

This process terminates when either  $f'_p = 0$  or *no*  $\text{in}(g_i)$  divides a monomial of  $f'_p$ ; the remainder  $f'$  is then the last  $f'_p$  produced.

We will illustrate this algorithm with an example.

**Example 2.2.4.** Choose the lexicographic term order  $\prec := \prec_{lex}$  on  $\mathbb{Q}[x, y]$  with  $x > y$ . Let  $f_1 := x^2y^2 - x$ ,  $f_2 := xy^3 + y$  and  $f := x^3y^2 - 2xy^4$ . We will show that  $x^2 - 2y^2$  is the remainder of division of  $f$  by  $f_1$  and  $f_2$ ; more precisely,

$$f = xf_1 + 2yf_2 + x^2 - 2y^2.$$

Note first that  $\text{in}_{\prec}(f_1) = x^2y^2$  and  $\text{in}_{\prec}(f_2) = xy^3$ .

Let  $f'_p := f$ . The maximal term of  $f'_p$  divisible by  $\text{in}_{\prec}(f_1)$  or  $\text{in}_{\prec}(f_2)$  is  $m := x^3y^2$ , since  $x^3y^2 = x(\text{in}_{\prec}(f_1))$ . Then we set

$$\begin{aligned} s_1 &:= 1, \\ m_1 &= \frac{m}{\text{in}_{\prec}(f_1)} = x. \end{aligned}$$

Now we let  $f'_p := f - m_1f_1 = f - xf_1 = 2xy^4 + x^2$ .

For the next step, we choose the term  $m := 2xy^4$  of  $f'_p$ , since it is divisible by  $\text{in}_{\prec}(f_2)$ . Then we set

$$\begin{aligned} s_2 &:= 2, \\ m_1 &= \frac{m}{\text{in}_{\prec}(f_2)} = \frac{2xy^4}{xy^3} = 2y. \end{aligned}$$

Now we let  $f'_p := f - xf_1 - 2yf_2 = x^2 - 2y^2$ . The algorithm stops here since no term of  $f'_p$  is divisible by either of the initial terms  $\text{in}_{\prec}(f_1)$ ,  $\text{in}_{\prec}(f_2)$ .

The last condition on the initial terms gives a motivation for the definition of Gröbner basis, and indicates why Gröbner bases are needed for ideal computations,

**Theorem 2.2.5** (Buchberger’s Criterion [8]). *The elements  $g_1, \dots, g_t \in I$  form a Gröbner basis of  $I$  if and only if  $h_{ij} = 0$  for all  $i$  and  $j$ , where  $h_{ij}$  is defined to be the remainder of division of the binomial*

$$S(g_i, g_j) := \frac{\text{in}(g_j)}{\text{GCD}(\text{in}(g_i), \text{in}(g_j))} g_i - \frac{\text{in}(g_i)}{\text{GCD}(\text{in}(g_i), \text{in}(g_j))} g_j$$

by the  $g_1, \dots, g_t$ . The binomial  $S(g_i, g_j)$  is called the S-pair of  $g_i$  and  $g_j$ .

In the following Chapters, this criterion will be used extensively. It supplies a first method for computing Gröbner bases:

**Algorithm 2.2.6** (Buchberger’s Algorithm [8]). Suppose that  $I$  is generated by  $\mathcal{G} := \{g_1, \dots, g_t\}$ . Compute the remainders  $h_{ij}$  as defined in the above Criterion. If all  $h_{ij} = 0$ , then  $\mathcal{G}$  is a Gröbner basis for  $I$ . If some  $h_{ij} \neq 0$ , then let  $\mathcal{G}' := \mathcal{G} \cup \{h_{ij}\}$  and repeat the process with  $\mathcal{G}'$ .

Since the ideal generated by the initial terms of elements in  $\mathcal{G}'$  is strictly larger than that generated by those of  $\mathcal{G}$ , the algorithm must terminate after finitely many steps, because  $S$  is a Noetherian ring.

It is a well-known result (eg. [34]) that even though there are infinitely many term orders, every ideal has only finitely many initial ideals, or, equivalently, a finite number of reduced Gröbner bases.

**Definition 2.2.7.** The union of all of the reduced Gröbner bases of  $I$  is called the *universal Gröbner basis* and denoted  $\mathcal{U}_I$ .

For a class of ideals called *toric ideals*, Gröbner bases have additional structure. (A standard reference on toric ideals is [34].) In this work, a toric ideal is any ideal that defines an affine or projective variety which is parametrized by monomials. To that end, fix a subset  $\mathcal{A} = \{a_1, \dots, a_n\}$  of  $\mathbb{Z}^d$ . The set  $\mathcal{A}$  determines a toric ideal in the following way: every vector  $u \in \mathbb{Z}^n$  can be written uniquely as  $u = u^+ - u^-$  where  $u^+$  and  $u^-$  are nonnegative and have disjoint support. More precisely, the nonzero of  $u^+$  are the positive entries of  $u$ , while the nonzero entries of  $u^-$  are the negatives of the negative entries of  $u$ . Such a vector  $u$  gives rise to a monomial

$$\mathbf{x}^u := \mathbf{x}^{u^+} - \mathbf{x}^{u^-} := x_1^{u_1^+} \dots x_n^{u_n^+} - x_1^{u_1^-} \dots x_n^{u_n^-} = \prod_{u_i > 0} x_i^{u_i} - \prod_{u_i < 0} x_i^{-u_i}$$

**Definition 2.2.8.** Considering  $\mathcal{A}$  as a  $d \times n$  integer matrix induces a parametrization of an affine variety  $Y := Y_{\mathcal{A}} \subset \mathbb{A}^n := K^n$  whose defining ideal is the toric ideal

$$I_{\mathcal{A}} := (x^{u^+} - x^{u^-} : Au = 0)$$

in the polynomial ring  $k[\mathbf{x}] := k[x_1, \dots, x_n]$ . If in addition the set  $\mathcal{A}$  is *graded*, i.e. the columns of  $\mathcal{A}$  lie in some hyperplane, then the toric ideal  $I_{\mathcal{A}}$  is homogeneous. In this case, the matrix  $\mathcal{A}$  defines a *projective* variety  $X := X_{\mathcal{A}} \subset \mathbb{P}^{n-1}$ .

We may write  $I_X$  for  $I_{\mathcal{A}}$ . The ideal  $I_{\mathcal{A}}$  is a prime ideal, and it is generated by binomials ([34]):

**Proposition 2.2.9.** *The toric ideal  $I_{\mathcal{A}}$  is generated by a (finite) set of binomials of the form  $x^{u^+} - x^{u^-}$  such that  $Au = 0$ .*

One way to calculate a generating set for  $I_{\mathcal{A}}$  given the matrix  $\mathcal{A}$  is the *saturation algorithm*:

**Definition 2.2.10.** Let the columns of the matrix  $B := \{b_i\}$  be a generating set of the lattice  $\ker_{\mathbb{Z}} \mathcal{A} := \{u \in \mathbb{Z}^n : Au = 0\}$ . The ideal

$$I_B := \left( \prod_{b_{ij} > 0} x_i^{b_{ij}} - \prod_{b_{ij} < 0} x_i^{-b_{ij}} \right)$$

is called the *lattice basis ideal* for  $I_{\mathcal{A}}$ . Moreover, the ideal  $I_{\mathcal{A}}$  is the *saturation* of  $I_B$ :

$$I_{\mathcal{A}} = I_B : (x_1 \dots x_n)^\infty := (f \in S : f \cdot (x_1 \dots x_n)^k \in I_B \text{ for some } k \in \mathbb{N})$$

Even though this is not the best way to calculate the generating set, we will see how the lattice basis ideal plays an essential role in our study of phylogenetic ideals in Chapter 4.

Let us return to Gröbner bases. In general, the structure of any Gröbner basis of  $I_{\mathcal{A}}$  can be quite complicated. However, if the initial ideal can be generated by *squarefree* monomials, then there are a few striking consequences for the variety. The following result is well-known to specialists.

**Lemma 2.2.11.** *Let  $I$  be a homogeneous toric ideal of a polynomial ring  $S$ . If, for some monomial order on  $S$ , the initial ideal of  $I$  is squarefree, then  $S/I$  is Cohen-Macaulay.*

*Proof.* The ideal  $I$  defines an affine toric variety  $Y$  and a projective toric variety  $X$ .  $X$  is projectively normal if and only if  $Y$  is normal. Theorem 13.15 in [34] says that, if for some term order  $\prec$  the initial ideal  $\text{in}_{\prec}(I)$  is squarefree, then  $X$  is projectively normal.

By assumption,  $S/I$  is isomorphic to a semigroup ring  $K[B]$  for a semigroup  $B \subset \mathbb{N}_0^d$ . Thus, using Proposition 13.5 in [34], we conclude that the semigroup  $B$  is normal. Hence, by a theorem of Hochster [24], the semigroup ring  $K[B]$  is Cohen-Macaulay.  $\square$

**Remark 2.2.12.** In fact, there is another nice consequence, for which we need more theory. See Proposition 5.2.4

In general, the degrees of elements in a Gröbner basis of an ideal  $I$  can be very large. Suppose that  $I$  has a Gröbner basis consisting of quadratic polynomials for some term order  $\prec$ . Then we say that the coordinate ring  $S/I$  is *G-quadratic*, and we have the following property (eg. see [13]):

**Proposition 2.2.13.** *If  $S/I$  is  $G$ -quadratic, then it is Koszul, while the converse does not hold.*

Even though the structure of Gröbner bases can be quite complicated, we expect some special properties to hold for toric ideals, since they are generated by binomials. Indeed, the steps (of forming S-pairs and calculating the remainder) in Buchberger's algorithm preserve the binomial structure! Therefore, *any Gröbner basis of a toric ideal consists of binomials*, and thus to describe the universal Gröbner basis, it suffices to consider binomials. Denote the universal Gröbner basis of the toric ideal  $I_{\mathcal{A}}$  by  $\mathcal{U}_{\mathcal{A}} := \mathcal{U}_{I_{\mathcal{A}}}$ . Good "approximations" of  $\mathcal{U}_{\mathcal{A}}$  are the circuits and the Graver basis:

**Definition 2.2.14.** A binomial  $x^{u^+} - x^{u^-} \in I_{\mathcal{A}}$  is called *primitive* if there is no  $x^{v^+} - x^{v^-} \in I_{\mathcal{A}}$  such that  $x^{v^+} | x^{u^+}$  and  $x^{v^-} | x^{u^-}$ . The set of all primitive binomials is called the *Graver basis* of  $I_{\mathcal{A}}$  and denoted by  $\mathcal{G}r_{\mathcal{A}}$ . A set of primitive binomials with minimal support is the set  $\mathcal{C}_{\mathcal{A}}$  of *circuits* of the ideal.

**Lemma 2.2.15** ([34]). *Every binomial in the universal Gröbner basis of a toric ideal is primitive. Every circuit is an element of some reduced Gröbner basis.*

Thus, we have  $\mathcal{C}_{\mathcal{A}} \subset \mathcal{U}_{\mathcal{A}} \subset \mathcal{G}r_{\mathcal{A}}$ . In general, both containments are proper. Obtaining an explicit description of either of these sets, or even a sharp degree bound for their elements, is a nontrivial task.



## Chapter 3

### Rational normal scrolls

There exists a general bound on the degrees of the elements of the universal Gröbner basis ([34]), however it is far too large for many specific examples. One might expect the sharp bound to be smaller for varieties that are special in some sense.

As mentioned in the introduction, rational normal scrolls are examples of varieties of *minimal degree*, that is, the varieties which attain the general lower bound  $\deg(X) \geq \text{codim}(X) + 1$  (Proposition 3.1.1). They have been classified ([18], Proposition 3.1.11) as quadratic hypersurfaces, rational normal scrolls, the Veronese surface in  $\mathbb{P}^5$ , and cones over these. The scrolls are the only family whose Gröbner bases were not precisely known.

The chapter is organized as follows. Sections 3.1 and 3.2 contains the necessary information about the defining ideals and parametrization of rational normal scrolls. In Section 3.3 we introduce colored partition identities and use them to characterize the Graver bases of the scrolls (Proposition 3.3.8), generalizing the result for rational normal curves in [21]. Section 3.4 contains the degree bounds. An important consequence of the sharp bound in Theorem 3.4.2 is that if  $X$  is any variety that can be obtained from a scroll by a sequence of projections to some of the coordinate hyperplanes, then the degree of the variety gives an upper bound on the degrees of elements in the universal Gröbner basis of its defining ideal  $I_X$ . In the final section, we conjecture that the universal Gröbner basis equals the Graver basis for any scroll, and discuss its consequences. We also derive the dimension of the state polytopes of scrolls.

#### 3.1 Background

A variety  $V \subset \mathbb{P}^n$  is called *non-degenerate* in  $\mathbb{P}^n$  if it is not contained in a projective space of smaller dimension; equivalently, if its defining ideal  $I_X$  contains no linear forms.

**Proposition 3.1.1.** *If  $V \subset \mathbb{P}^n$  is a non-degenerate variety, then*

$$\deg V \geq \text{codim} V + 1 = n - \dim V + 1.$$

To prove this, we need to use another theorem:

**Theorem 3.1.2** (Bertini's Theorem). *Let  $V \subset \mathbb{P}^n$  be an irreducible variety of dimension  $d \geq 1$  and  $H \subset \mathbb{P}^n$  a sufficiently general hyperplane. Then:*

- (i) *If  $V$  is non-degenerate, then the hyperplane section  $V \cap H$  is non-degenerate in  $H$ .*

(ii)  $V \cap H$  is always reduced and also irreducible (i.e., its defining ideal is prime), provided that  $d \geq 2$ .

We will omit the proof of this well-known result.

*Proof of Proposition 3.1.1.* Assume  $\dim V = d = 1$ , i.e.  $V$  is a curve (if  $d = 0$ ,  $V$  is a point so the claim is trivial). Then  $V \cap H$  is a (reduced) set of points spanning  $H \cong \mathbb{P}^{n-1}$ , as non-degeneracy implies that the points must span the whole hyperplane. Hence  $\deg(V \cap H) = |\text{points in } V \cap H| \geq n$ , as claimed. Finally, if  $d > 1$ , then we conclude by induction because  $\text{codim}_H(V \cap H) = \text{codim}_{\mathbb{P}^n} V$  and  $\deg V \cap H = \deg V$ .  $\square$

Now we are ready to make the crucial definition:

**Definition 3.1.3.** A variety  $V$  of *minimal degree* is an irreducible variety that is either linear (of degree 1) or has degree  $s - \dim V + 1$ , where  $s$  is the dimension of the linear span of  $V$ :  $s + 1 := \dim[S/I_V]_1 = h_{S/I_V}(1)$ . Non-degeneracy implies that  $s = n$ .

For example, consider a non-degenerate hypersurface. Non-degeneracy rules out linear equations, so the degree must be at least two. Thus a hypersurface is a variety of minimal degree if and only if its degree is at least two.

Another example of varieties of minimal degree are rational normal curves.

**Definition 3.1.4.** The image of the map

$$\begin{aligned} \nu : \mathbb{P}^1 &\rightarrow \mathbb{P}^n \\ (s : t) &\mapsto (s^n : s^{n-1}t : \dots : t^n) \end{aligned}$$

is called the (*standard*) *rational normal curve (RNC)*  $C$  in  $\mathbb{P}^n$ . More generally, a rational normal curve is any curve that is isomorphic to  $C$  by a linear change of coordinates.

To describe a parametrization of a variety is equivalent to describing its vanishing ideal. The ideals of rational normal curves have a very special structure. We will omit the proof of this well-known result, as well as subsequent results in this section. They can be found, for example, in [18].

**Proposition 3.1.5.** Let  $C \subset \mathbb{P}^n$  be the standard rational normal curve, and let

$$M_n := \begin{bmatrix} x_1 & x_2 & \dots & x_n \\ x_2 & x_3 & \dots & x_{n+1} \end{bmatrix}.$$

Then:

- (i)  $C$  is non-degenerate.
- (ii)  $I_C = I_2(M_n)$ , the ideal of 2-minors of the matrix  $M_n$ .
- (iii)  $I_C$  is a prime ideal.

(iv)  $C$  is a variety of minimal degree.

A natural question to ask is what varieties are defined by 2-minors of matrices whose structure is a generalization of that of  $M_n$ . To this end, let us define a 1-generic matrix.

**Definition 3.1.6.** Let  $M \in S^{p,q}$  be a matrix of linear forms. Then:

1. A *generalized row* of  $M$  is a nontrivial scalar linear combinations of the rows of  $M$ . Similarly, one defines a *generalized column*.
2.  $M$  is said to be 1-generic if the entries in every generalized row or column of  $M$  are linearly independent.

For example,  $M_n$  is 1-generic. In general, 1-generic matrices generalize  $M_n$ :

**Proposition 3.1.7.** Let  $M \in S^{2,k}$  be 1-generic, where  $n \geq k \geq 2$ , and the entries of  $m$  span  $[S]_1$ . Set  $d := n + 1 - k$ . Then there exist positive integers  $a_1, \dots, a_d$  such that  $a_1 + \dots + a_d = n + 1$  and the matrix

$$M_{\mathbf{a}} := [M_{a_1} \mid M_{a_2} \mid \dots \mid M_{a_d}]$$

where  $M_{a_i} \in S^{2,a_i}$  is defined as in Proposition 3.1.5 in the variables  $x_j$  with

$$a_1 + \dots + a_{i-1} + i - 1 \leq j \leq a_2 + \dots + a_i + i - 1,$$

such that  $M$  is conjugate to  $M_{\mathbf{a}}$ .

For example, if  $\mathbf{a} = (3, 2, 1)$ , then  $d = 3$ ,  $n = 8$ , and

$$M_{\mathbf{a}} = \begin{bmatrix} x_1 & x_2 & x_3 & x_5 & x_6 & x_8 \\ x_2 & x_3 & x_4 & x_6 & x_7 & x_9 \end{bmatrix}.$$

**Lemma 3.1.8.** If  $M \in S^{p,q}$  is a 1-generic matrix with  $p \leq q$ , then the ideal of maximal minors  $I_p(M)$  is a prime ideal.

It turns out that for  $p = 2$ , these are precisely the ideals that we are interested in:

**Definition 3.1.9.** A *rational normal scroll* is a variety  $\mathcal{S} \subset \mathbb{P}^n$  that is defined by  $I_2(M)$  where  $M \in S^{2,k}$  is a 1-generic matrix with  $k \leq n$ .  
If

$$M := [M_{n_1-1} \mid M_{n_2-1} \mid \dots \mid M_{n_c-1}], \text{ and } M_{n_j} := \begin{bmatrix} x_{j,1} & \dots & x_{j,n_j-1} \\ x_{j,2} & \dots & x_{j,n_j} \end{bmatrix},$$

then we denote the scroll defined by  $I_M$  by  $\mathcal{S} := \mathcal{S}(n_1 - 1, \dots, n_c - 1)$ .

Note that if  $c = 1$ , then the 2-minors of the matrix above give the defining ideal of a rational normal curve  $S(n - 1)$  in  $\mathbb{P}^{n-1}$  ([18]).

**Corollary 3.1.10.** *Assume that  $d + n_1 - 1 + \dots + n_c - 1 =: n + 1$ . Then*

$$\dim(\mathcal{S}(n_1 - 1, \dots, n_c - 1)) = d$$

and

$$\deg(\mathcal{S}(n_1 - 1, \dots, n_c - 1)) = n - d + 1.$$

*In particular, each rational normal scroll of dimension  $d$  is a variety of minimal degree.*

Finally we arrive at the crucial theorem:

**Theorem 3.1.11** (Del Pezzo 1886; Bertini 1907.; see [18]).  *$X \subset \mathbb{P}^n$  is a non-degenerate variety of minimal degree if and only if  $X$  is (up to a change of coordinates) a cone over one of the following varieties:*

1. *quadratic hypersurface,*
2. *rational normal scroll  $\mathcal{S}$ ,*
3. *the Veronese surface in  $\mathbb{P}^5$ , which is defined as the image of the map*

$$\begin{aligned} \nu : \mathbb{P}^2 &\rightarrow \mathbb{P}^5 \\ (s : t : w) &\mapsto (s^2 : st : sw : t^2 : tw : w^2) \end{aligned}$$

Thus, to study Gröbner bases of varieties of minimal degree, we need to focus on the rational normal scrolls, since they are the only infinite family whose Gröbner bases are not all known.

### 3.2 Parametrization of Scrolls

We know that the defining ideal of every rational normal scroll is given by the 2-minors of the matrix  $M$  as defined in the previous section. The ideal  $I_{\mathcal{S}}$  is generated by binomials and it is thus a toric ideal. In order to study the combinatorial properties of its Gröbner bases, we need to find the parametrization matrix  $\mathcal{A}$  corresponding to each scroll.

**Lemma 3.2.1.**  *$I_{\mathcal{S}} = \ker \varphi$ , where  $\varphi(x_{j,i}) = [v_1^1, \dots, v_j^1, v_{j+1}^0, \dots, v_c^0, t^i]^T$  for  $1 \leq j \leq c$ . That is, the matrix  $\mathcal{A}$  that encodes the parametrization of the scroll  $\mathcal{S}$  is*

$$\mathcal{A} = \begin{bmatrix} 1 & \dots & 1 & 1 & \dots & 1 & \dots & 1 & \dots & 1 \\ 0 & \dots & 0 & 1 & \dots & 1 & \dots & 1 & \dots & 1 \\ \vdots & & & & & & & & & \vdots \\ 0 & \dots & 0 & 0 & \dots & 0 & \dots & 1 & \dots & 1 \\ 1 & 2 \dots & n_1 & 1 & \dots & n_2 & \dots & 1 & \dots & n_c \end{bmatrix}.$$

*Proof.* Indeed, let the generators of  $I_{\mathcal{S}}$  be the minors

$$m_{i,j,k,l} := x_{i,k}x_{j,l+1} - x_{j,l}x_{i,k+1}$$

for  $1 \leq i, j \leq c$ ,  $1 \leq k \leq n_i - 1$ , and  $1 \leq l \leq n_j - 1$ . (Note that we allow  $i = j$  and  $k = l$ .) Then the exponent vector of  $m_{i,j,k,l}$  is

$$v_{i,j,k,l} = [0, \dots, 0, 1, 0, \dots, 0, -1, 0, \dots, 0, -1, 0, \dots, 0, 1, 0, \dots, 0]^T$$

where the positive entries are in columns  $n_1 + \dots + n_{i-1} + k$  and  $n_1 + \dots + n_{j-1} + l + 1$ , while the negative entries are in columns  $n_1 + \dots + n_{j-1} + l$  and  $n_1 + \dots + n_{i-1} + k + 1$ . (If  $i = j$  and  $k = l$ , then the two locations for the negative entries coincide; in that case, the negative entry is  $-2$ .) Denote by  $\mathcal{A}_c$  the  $c^{\text{th}}$  column of  $\mathcal{A}$ . Then clearly

$$\mathcal{A}_{n_1 + \dots + n_{i-1} + k} + \mathcal{A}_{n_1 + \dots + n_{j-1} + l + 1} = \mathcal{A}_{n_1 + \dots + n_{j-1} + l} + \mathcal{A}_{n_1 + \dots + n_{i-1} + k + 1}$$

since

$$\begin{bmatrix} 1 \\ \vdots \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \\ k \end{bmatrix} + \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ l + 1 \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \\ k + 1 \end{bmatrix} + \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ l \end{bmatrix}.$$

Thus  $m_{i,j,k,l} \in I_{\mathcal{A}}$  for each generator  $m_{i,j,k,l}$  of  $I_{\mathcal{S}}$ .

In addition, the matrix  $\mathcal{A}$  has full rank; thus the dimension of the variety it parametrizes is  $\text{rank } \mathcal{A} - 1 = c$ . But this is precisely the dimension of the scroll  $\mathcal{S}$ .  $\square$

**Example 3.2.2.** The ideal of the scroll  $\mathcal{S}(3, 2)$  is the toric ideal  $I_{\mathcal{A}_{\mathcal{S}(3,2)}}$  where

$$\mathcal{A}_{\mathcal{S}(3,2)} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 1 & 2 & 3 \end{bmatrix}.$$

### 3.3 Colored partition identities and Graver bases

Let us begin by generalizing the definitions of *primitive partition identities* (ppi's) and *homogeneous ppi's* from Chapter 6 of [34].

**Definition 3.3.1.** A **colored partition identity** (or a **cpi**) in the colors  $(1), \dots, (c)$  is an identity of the form

$$\begin{aligned} a_{1,1} + \dots + a_{1,k_1} + a_{2,1} + \dots + a_{2,k_2} + \dots + a_{c,1} + \dots + a_{c,k_c} = \\ b_{1,1} + \dots + b_{1,s_1} + b_{2,1} + \dots + b_{2,s_2} + \dots + b_{c,1} + \dots + b_{c,s_c}, \end{aligned} \quad (*)$$

where  $1 \leq a_{p,j}, b_{p,j} \leq n_p$  are positive integers for all  $j$ ,  $1 \leq p \leq c$  and some positive integers  $n_1, \dots, n_c$ .

If  $c = 1$  then this is precisely the definition of the usual partition identity with  $n = n_1$ .

**Remark 3.3.2.** A cpi in  $c$  colors with  $n_1, \dots, n_c$  as above is a partition identity (in one color) with *largest part*  $n = \max\{n_1, \dots, n_c\}$ .

**Example 3.3.3.** Denote by  $i_r$  the number  $i$  colored red, and by  $i_b$  the number  $i$  colored blue. Then

$$1_r + 4_r + 3_b = 5_b + 1_b + 2_r$$

is a colored partition identity with two colors, with  $n_1 = 4$  and  $n_2 = 5$ . Erasing the coloring gives  $1 + 4 + 3 = 5 + 1 + 2$ , a (usual) partition identity with largest part  $n = 5$ .

**Definition 3.3.4.** A colored partition identity (\*) is a **primitive** cpi (or a **pcpi**) if there is no proper sub-identity  $a_{-,i_1} + \dots + a_{-,i_l} = b_{-,j_1} + \dots + b_{-,j_t}$ , with  $1 \leq l + t < k_1 + \dots + k_c + s_1 + \dots + s_c$ , which is a cpi.

A cpi is called **homogeneous** if  $k_1 + \dots + k_c = s_1 + \dots + s_c$ . If  $k_j = s_j$  for  $1 \leq j \leq c$ , then it is called **color-homogeneous**. The **degree** of a pcpi is the number of summands  $k_1 + \dots + k_c + s_1 + \dots + s_c$ .

Note that color-homogeneity implies homogeneity, and that a homogeneous pcpi need not be primitive in the inhomogeneous sense.

**Example 3.3.5.** Here is a list of all primitive color-homogeneous partition identities with  $c = 2$  colors and  $n_1 = n_2 = 3$ :

$$\begin{aligned} 1_1 + 3_1 &= 2_1 + 2_1 \\ 1_1 + 2_2 &= 2_1 + 1_2 \\ 1_1 + 1_1 + 3_2 &= 2_1 + 2_1 + 1_2 \\ 1_1 + 3_2 &= 2_1 + 2_2 \\ 2_1 + 3_2 &= 3_1 + 2_2 \\ 2_1 + 2_2 &= 3_1 + 1_2 \\ 1_1 + 3_2 &= 3_1 + 1_2 \\ 1_2 + 3_2 &= 2_2 + 2_2 \\ 1_1 + 3_2 + 3_2 &= 3_1 + 2_2 + 2_2 \\ 1_1 + 2_2 + 2_2 &= 3_1 + 1_2 + 1_2 \\ 2_1 + 2_1 + 3_2 &= 3_1 + 3_1 + 1_2. \end{aligned}$$

We are now ready to relate the ideals of scrolls and the colored partition identities.

**Lemma 3.3.6.** *A binomial  $x_{1,a_{1,1}} \dots x_{1,a_{1,k_1}} \dots x_{c,a_{c,1}} \dots x_{c,a_{c,k_c}} - x_{1,b_{1,1}} \dots x_{c,b_{c,s_c}}$  is in the ideal  $I_{AS(n_1-1, \dots, n_c-1)}$  if and only if (\*) is a color-homogeneous cpi.*

*Proof.* This follows easily from the definitions and Lemma 3.2.1. □

**Example 3.3.7.** Let  $c = 2$ . Then

$$A := \mathcal{A}_{\mathcal{S}(n_1-1, n_2-1)} = \begin{bmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ 0 & \dots & 0 & 1 & \dots & 1 \\ 1 & \dots & n_1 & 1 & \dots & n_2 \end{bmatrix}$$

and

$$I_A = I_2 \begin{bmatrix} x_{1,1} & \dots & x_{1,n_1-1} & x_{2,1} & \dots & x_{2,n_2-1} \\ x_{1,2} & \dots & x_{1,n_1} & x_{2,2} & \dots & x_{2,n_2} \end{bmatrix}.$$

Then  $x_{1,a_{1,1}} \dots x_{1,a_{1,k_1}} x_{2,a_{2,1}} \dots x_{2,a_{2,k_2}} - x_{1,b_{1,1}} \dots x_{1,b_{1,s_1}} x_{2,b_{2,1}} \dots x_{2,b_{2,s_2}} \in I_A$  if and only if

$$\begin{bmatrix} v_1^{k_1+k_2} \\ v_2^{0+k_2} \\ t^{a_{1,1}+\dots+a_{2,k_2}} \end{bmatrix} = \begin{bmatrix} v_1^{s_1+s_2} \\ v_2^{0+s_2} \\ t^{b_{1,1}+\dots+b_{2,s_2}} \end{bmatrix}$$

if and only if  $k_1 + k_2 = s_1 + s_2$ ,  $k_2 = s_2$ , and

$$a_{1,1} + \dots + a_{1,k_1} + a_{2,1} + \dots + a_{2,k_2} = b_{1,1} + \dots + b_{1,s_1} + b_{2,1} + \dots + b_{2,s_2}.$$

But this is equivalent to the definition of a color-homogeneous pcpi.

The Lemmas above imply the following characterization of the Graver bases of rational normal scrolls.

**Proposition 3.3.8.** *The Graver basis elements for the scroll  $\mathcal{S}(n_1 - 1, \dots, n_c - 1)$  are precisely the color-homogeneous primitive colored partition identities of the form (\*).*

*Proof.* With all the tools in hand, it is not difficult to check that the binomial in the ideal of the scroll is primitive if and only if the corresponding colored partition identity is primitive.  $\square$

If  $c = 1$ , this is just the observation in Chapter 6 of [34] which states that the primitive elements in the ideal of a rational normal curve are in one-to-one correspondance with the homogeneous primitive partition identities.

### 3.4 Degree bounds

Now we can generalize the degree bound given in [34] for the rational normal curves:

**Theorem 3.4.1** ([34]). *The degree of any primitive binomial in the ideal of the rational normal curve  $\mathcal{S}(n - 1) \subset \mathbb{P}^{n-1}$  is at most  $n - 1$ .*

Our degree bound is sharp. Moreover, the maximal degree is always attained by a circuit, which is quite a remarkable property.

In what follows, by a *subscroll* of  $\mathcal{S}(n_1 - 1, \dots, n_c - 1)$  we mean a scroll  $\mathcal{S}' := \mathcal{S}(n'_1 - 1, \dots, n'_c - 1)$  such that  $n'_i \leq n_i$  for each  $i$ . Clearly,  $I_{\mathcal{S}'}$  can be obtained from  $I_{\mathcal{S}}$  by eliminating variables, that is,  $I_{\mathcal{S}'} = I_{\mathcal{S}} \cap R$  where  $R$  is a subring of  $S$  with less variables.

**Theorem 3.4.2.** Let  $\mathcal{S} := \mathcal{S}(n_1 - 1, \dots, n_c - 1)$  for  $c \geq 2$ . Let  $P$  and  $Q$  be the indices such that

$$n_P = \max\{n_i : 1 \leq i \leq c\}$$

and

$$n_Q = \max\{n_j : 1 \leq j \leq c, j \neq P\}.$$

Then the degree of any primitive binomial in  $I_{\mathcal{S}}$  is bounded above by

$$n_P + n_Q - 2.$$

This bound is sharp exactly when  $n_P - 1$  and  $n_Q - 1$  are relatively prime.

More precisely, the primitive binomials in  $I_{\mathcal{S}}$  have degree at most

$$u + v - 2,$$

where  $u$  and  $v$  are maximal integers such that  $\mathcal{S}(n'_1 - 1, \dots, n'_c - 1)$  is a subscroll of  $\mathcal{S}$  with  $n'_i = u$  and  $n'_j = v$  for some  $1 \leq i, j \leq c$ , and subject to  $(u - 1, v - 1) = 1$ . This degree bound is sharp; there is always a circuit having this degree. For any number of colors  $c$ , such a maximal degree circuit is two-colored.

Before proving the Theorem, let us look at an example.

- Example 3.4.3.** 1. Consider the scroll  $\mathcal{S}(5, 6)$ . Here  $n_P - 1 = 6$  and  $n_Q - 1 = 5$ , and since they are relatively prime, the sharp degree bound is  $5 + 6 = 11$ .
2. On the other hand, if  $\mathcal{S} := \mathcal{S}(4, 4, 2, 2)$ , then  $n_P - 1 = n_Q - 1 = 4$  so we look for a subscroll  $\mathcal{S}' := \mathcal{S}(4, 3, 2, 2)$ . Then  $u - 1 = 4$  and  $v - 1 = 3$ , and the degree of any primitive element is at most 7.
3. If  $\mathcal{S} := \mathcal{S}(5, 5, 5)$ , then  $n_P - 1 = n_Q - 1 = 5$ . The desired subscroll is  $\mathcal{S}' := \mathcal{S}(5, 4, 4)$  so that the degree bound is  $u - 1 + v - 1 = 5 + 4 = 9$ .

*Proof of Theorem 3.4.2.* Let  $x_{1,a_{1,1}} \dots x_{c,a_{c,k_c}} - x_{1,b_{1,1}} \dots x_{c,b_{c,k_c}}$  be a primitive binomial in  $I_{\mathcal{S}}$ . Consider the corresponding color-homogeneous pcpi:

$$\begin{aligned} a_{1,1} + \dots + a_{1,k_1} + a_{2,1} + \dots + a_{2,k_2} + \dots + a_{c,1} + \dots + a_{c,k_c} = \\ b_{1,1} + \dots + b_{1,k_1} + b_{2,1} + \dots + b_{2,k_2} + \dots + b_{c,1} + \dots + b_{c,k_c}. \end{aligned} \quad (**)$$

Note that the number of terms on either side of (\*\*) equals the degree of the binomial. We shall first show that  $k_1 + \dots + k_c \leq n_P + n_Q - 2$  holds for (\*\*).

Let  $d_{i,j} = a_{i,j} - b_{i,j}$  be the differences in the  $i^{\text{th}}$ -color entries for  $1 \leq j \leq k_i$ ,  $1 \leq i \leq c$ . Then

$$\sum_{\substack{1 \leq i \leq c \\ 1 \leq j \leq k_i}} d_{i,j} = 0.$$

Separating positive and negative terms gives an inhomogeneous pcpi  $\sum d_{i,j}^+ = \sum d_{i,j}^-$ . Indeed, if it is not primitive, then there would be a subidentity in (\*\*), contradicting



its primitivity. Note that an inhomogeneous pcpi is defined to be a ppi with arbitrary coloring. Therefore, the sum-difference algorithm from the proof of Theorem 6.1. in [34] can be applied. For completeness, let us recall the algorithm.

Set  $x := 0$ ,  $\mathcal{P} := \{d_{i,j}^+\}$ ,  $\mathcal{N} := \{d_{i,j}^-\}$ .  
 While  $\mathcal{P} \cup \mathcal{N}$  is non-empty do  
   if  $x \geq 0$   
     then select an element  $\nu \in \mathcal{N}$ , set  $x := x - \nu$  and  $\mathcal{N} := \mathcal{N} \setminus \{\nu\}$   
     else select an element  $\pi \in \mathcal{P}$ , set  $x := x + \pi$  and  $\mathcal{P} := \mathcal{P} \setminus \{\pi\}$ .

The number of terms in the pcpi is bounded above by the number of values  $x$  can obtain during the run of the algorithm. Primitivity ensures that no value is reached twice. Let

$$D_{i,+} := \max_j \{d_{i,j} : d_{i,j} > 0\}$$

and

$$D_{i,-} := \max_j \{-d_{i,j} : d_{i,j} < 0\}.$$

Then by Corollary 6.2 in [34],  $k_1 + \dots + k_c \leq \max_i \{D_{i,+}\} + \max_i \{D_{i,-}\}$ . Let

$$D_+ := \max_i \{D_{i,+}\}$$

and

$$D_- := \max_i \{D_{i,-}\}.$$

Suppose  $D_+$  and  $D_-$  occur in colors  $P$  and  $Q$ , respectively, so that  $D_+ = a_P - b_P$ , and  $D_- = b_Q - a_Q$ . Then the sequence of inequalities

$$1 + D_+ + 1 \leq 1 + D_+ + b_P = 1 + a_P \leq 1 + n_P \leq a_Q + n_P = b_Q - D_- + n_P \leq n_Q - D_- + n_P$$

implies that

$$D_+ + D_- \leq n_P + n_Q - 2,$$

and the degree bound follows.

The maximum degree occurs when there is equality in the above sequence of inequalities, and  $x$  reaches every possible value during the run of the algorithm. Following the argument of Sturmfels in the proof of the same theorem (6.1. in [34]), it can be easily checked that the inhomogeneous pcpi  $\sum d_{i,j} = 0$  is of the form

$$\underbrace{D_+ + \dots + D_+}_{D_- \text{ terms}} = \underbrace{D_- + \dots + D_-}_{D_+ \text{ terms}}.$$

In addition,

$$1 + D_+ + 1 = 1 + D_+ + b_P = 1 + a_P = 1 + n_P = a_Q + n_P = b_Q - D_- + n_P = n_Q - D_- + n_P$$

implies that  $b_P = 1$ ,  $a_P = n_P$ ,  $a_Q = 1$ , and  $b_Q = n_Q$ . Therefore, the maximal degree identity  $\sum d_{i,j} = 0$  provides that (\*\*\*) is of the following form:

$$\underbrace{1_P + \dots + 1_P}_{n_Q-1 \text{ terms}} + \underbrace{n_Q + \dots + n_Q}_{n_P-1 \text{ terms}} = \underbrace{1_Q + \dots + 1_Q}_{n_P-1 \text{ terms}} + \underbrace{n_P + \dots + n_P}_{n_Q-1 \text{ terms}},$$

where  $1_P$  denotes the number 1 colored using the color  $P$ . This colored partition identity is primitive if and only if there does not exist a proper subidentity, which in turn holds if and only if  $n_P - 1$  and  $n_Q - 1$  are relatively prime. Indeed, if  $n_P - 1 = zy$  and  $n_Q - 1 = zw$  for some  $z, y, w \in \mathbb{N}$ , then there is a subidentity of the form

$$\underbrace{1_P + \cdots + 1_P}_w + \underbrace{n_Q + \cdots + n_Q}_y = \underbrace{1_Q + \cdots + 1_Q}_y + \underbrace{n_P + \cdots + n_P}_w.$$

Furthermore, assume that  $n_P - 1$  and  $n_Q - 1$  are relatively prime. Then the exponent vector of the binomial corresponding to the maximal degree identity has support of cardinality four. It is thus a circuit for any  $c \geq 2$ . Clearly, it is a two-colored circuit, regardless of the number of colors  $c$  in our scroll  $\mathcal{S}$ .

Finally, if  $n_P - 1$  and  $n_Q - 1$  are not relatively prime, the degree  $n_Q + n_P - 2$  cannot be attained by a primitive binomial. In that case, we may simply eliminate one of the variables associated with color  $P$  to obtain a smaller scroll, say  $\mathcal{S}' := \mathcal{S}(n_1 - 1, \dots, n_P - 2, \dots, n_c - 1)$ , whose defining ideal is embedded in that of  $\mathcal{S}$  (that is, we let  $u := n_P - 1$  and  $v := n_Q$ ). Clearly, primitive binomials from  $I_{\mathcal{S}'}$  lie in  $I_{\mathcal{S}}$  (for example, see [34], Proposition 4.13). If  $u - 1$  and  $v - 1$  are relatively prime, then we have the smaller bound for the degree:  $n_P + n_Q - 3$ . If not, we continue eliminating variables until the condition is satisfied.

This completes the proof.  $\square$

**Remark 3.4.4.** In view of the comment on p.36 of [34], it is interesting to note that in the case of varieties of minimal degree, the maximum degree of any Graver basis element is attained by a circuit. This is not true in general.

Now the following is trivial.

**Corollary 3.4.5.** *The degree of any binomial in the Graver basis (and the universal Gröbner basis) of any rational normal scroll is bounded above by the degree of the scroll.*

In addition, this also gives the upper bound for the degrees of any element in the universal Gröbner basis of any variety whose parametrization can be embedded into that of a scroll, generalizing Corollary (6.5) from [34].

**Corollary 3.4.6.** *Let  $X$  be any toric variety that can be obtained from a scroll by a sequence of projections to some of the coordinate hyperplanes. Then the degree of an element of any reduced Gröbner basis of  $I_X$  is at most the degree of the toric variety  $X$ .*

*Proof.* The claim follows from degree-preserving coordinate projections and the elimination property of the universal Gröbner basis. The variety  $X = X_{\mathcal{A}}$  is parametrized by

$$\mathcal{A} = \begin{bmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 & \cdots & 1 & \cdots & 1 \\ 0 & \cdots & 0 & 1 & \cdots & 1 & \cdots & 1 & \cdots & 1 \\ \vdots & & & & & & & & & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \cdots & 1 & \cdots & 1 \\ i_{1,1} & i_{1,2} \cdots & i_{1,r_1} & i_{2,1} & \cdots & i_{2,r_2} & \cdots & i_{c,1} & \cdots & i_{c,r_c} \end{bmatrix}$$

In what follows, we may assume that  $1 = i_{k,1} < \dots < i_{k,r_k} := n_k$  for  $1 \leq k \leq c$ . Then  $X$  can be obtained by coordinate projections from the scroll  $\mathcal{S} := \mathcal{S}(n_1-1, \dots, n_c-1)$ , parametrized by  $\mathcal{A}_S$  as before. The degree of the toric variety  $X_{\mathcal{A}}$  is the normalized volume of the polytope formed by taking the convex hull of the columns of  $\mathcal{A}$ . But by construction we have  $\text{vol}(\text{conv}(\mathcal{A})) = \text{vol}(\text{conv}(\mathcal{A}_S))$ , thus the two varieties have the same degree.

Suppose  $x^u - x^v$  is in some reduced Gröbner basis of  $I_X$ . Then Proposition 4.13. and Lemma 4.6. in [34] provide that  $x^u - x^v \in \mathcal{U}_{\mathcal{A}} \subset \mathcal{U}_{\mathcal{A}_S} \subset \mathcal{G}r_{\mathcal{A}_S}$ . Applying Corollary 3.4.5 completes the proof.  $\square$

**Remark 3.4.7.** In particular, note that this degree bound (which equals the degree of the scroll,  $n_1 + \dots + n_c - c$ ) is always better than the general one given for toric ideals in [34], Corollary 4.15, which equals  $1/2(c+2)(n_1 + \dots + n_c - c - 1)D(\mathcal{A})$  where  $D(\mathcal{A})$  is the maximum over all  $(c+1)$ -minors of  $\mathcal{A}$ .

Let us conclude this section by listing the number of all elements in the Graver basis of some small scrolls, sorted by degree of the binomial. The entries in this table have been obtained using the software 4ti2 [42], which was essential in this project.

Scroll	Degrees									
	2	3	4	5	6	7	8	9	10	11
S(2,2)	7	4								
S(2,2,2)	18	24								
S(4)	7	7	2							
S(3,2)	12	16	4	1						
S(3,2,2)	26	58	22	4						
S(3,3)	20	40	18	4						
S(3,3,2,2)	59	242	208	36						
S(4,2)	19	39	20	4						
S(4,3)	30	86	58	15	2	1				
S(4,4)	44	166	146	52	12	4				
S(4,3,2,2)	75	391	524	176	6	1				
S(5,2)	28	83	72	32	4	1				
S(6,2)	40	157	182	95	28	4				
S(5,3)	42	166	174	78	16	6	1			
S(6,3)	57	290	412	210	62	14	2			
S(7,2)	55	280	432	294	130	46	4	1		
S(5,5,5)	204	2526	10002	10404	5088	1764	444	78		
S(6,5)	105	813	1678	1136	454	149	42	12	2	1

### 3.5 Universal Gröbner bases

The Graver basis is a good approximation to the universal Gröbner basis, but they are not equal in general. However, extensive computations using 4ti2 ([42]) show evidence supporting the following conjecture:

**Conjecture 3.5.1.**  $\mathcal{U}_{\mathcal{A}} = \mathcal{G}r_{\mathcal{A}}$  for the defining matrix  $\mathcal{A}$  of any rational normal scroll.

Note that the defining ideal of  $\mathcal{S} := \mathcal{S}(n_1 - 1, \dots, n_c - 1)$  is contained in the defining ideal of the scroll

$$\mathcal{S}(n_1 - 1, \dots, n_c - 1, \underbrace{1, \dots, 1}_l)$$

for any  $l$ . Define  $\mathcal{S}'$  to be any such scroll, where  $l$  is chosen so that the inequality

$$c + l + 3 > 2(n_P + n_Q - 2 - j_0)$$

is satisfied, where  $n_P + n_Q - 2 - j_0$  is the degree bound for the scroll  $\mathcal{S}'$  from Theorem 3.4.2. This puts a restriction on *the size of the support* of any primitive binomial. Let  $f \in \mathcal{G}r_{\mathcal{A}}$ . Then  $f \in I_{\mathcal{A}'}$  where  $\mathcal{A}' := \mathcal{A}_{\mathcal{S}'}$ . The primitivity of  $f$  implies  $f \in \mathcal{G}r_{\mathcal{A}'}$ . If the conjecture is true for the scroll  $\mathcal{S}'$ , then  $f$  lies in the universal Gröbner basis of the ideal  $I_{\mathcal{A}'}$ , and hence in the universal Gröbner basis of  $I_{\mathcal{A}}$ .

Therefore, to prove this conjecture, it suffices to prove a weaker one:

**Conjecture 3.5.2.**  $\mathcal{U}_{\mathcal{A}} = \mathcal{G}r_{\mathcal{A}}$  for rational normal scrolls of sufficiently high dimension.

Recently, Hemmecke and Nairn in [23] stated that if the universal Gröbner basis and Graver basis of  $I_{\mathcal{A}}$  coincide, then the Gröbner and Graver complexities of  $\mathcal{A}$  are equal. We plan to study the higher Lawrence configurations of the rational normal scrolls.

Next, we consider state polytopes of rational normal scrolls. Knowing a universal Gröbner basis of  $I_{\mathcal{A}}$  is equivalent to knowing its *state polytope* ([34]). It is defined to be any polytope whose normal fan coincides with the *Gröbner fan* of the ideal. The cones of the Gröbner fan correspond to the reduced Gröbner bases  $\mathcal{G}_{\prec}$  of  $I_{\mathcal{A}}$ . In addition, the Gröbner fan is a refinement of the secondary fan  $\mathcal{N}(\Sigma(\mathcal{A}))$ , which classifies equivalence classes of lifting functions giving a particular regular triangulation of the point configuration  $\mathcal{A}$ .

**Theorem 3.5.3.** *The dimension of the state polytope of a rational normal scroll is one less than the degree of the scroll:*

$$\dim \text{State}(I_{\mathcal{S}(n_1-1, \dots, n_c-1)}) = n_1 + \dots + n_c - c - 1.$$

*Proof.* Eliminating variables results in taking faces of the state polytope. Thus the state polytope for the scroll  $\mathcal{S}(n_1 - 1)$  is a face of that of  $\mathcal{S}(n_1 - 1, 1)$ , which in turn is a face of the state polytope of  $\mathcal{S}(n_1 - 1, 2)$ , etc. so that each time we add a column to the parametrization matrix  $\mathcal{A}_{\mathcal{S}}$ , the dimension of the state polytope grows by at least one. The ideal of the scroll  $\mathcal{S}(1, \dots, 1)$  is just the ideal of 2-minors of a generic  $2 \times c$  matrix. In this case, the minors form a universal Gröbner basis for the ideal,

which is also a reduced Gröbner basis of the ideal with respect to every term order ([34]). Hence, the state polytope is a Minkowski sum of the Newton polytopes of the minors (Cor. 2.9. in [34]), a permutohedron  $\Pi_{2,c}$  ([4],[38]). Its dimension is  $c - 1$ . By induction,

$$\dim \text{State}(\mathcal{S}(n_1 - 1, \dots, n_c - 1)) \geq n_1 - 2 + n_2 - 1 + \dots + n_c - 1 = \sum n_i - c - 1.$$

On the other hand, the ideal of the scroll is homogeneous with respect to the grading given by all the rows of  $\mathcal{A}_{\mathcal{S}}$ . There are  $c + 1$  independent rows, thus the vertices of the state polytope lie in  $c + 1$  hyperplanes, and the claim follows.  $\square$

Let us conclude this chapter with an example.

**Example 3.5.4.** Let  $S$  be the scroll  $\mathcal{S}(5,6)$ . Its defining ideal  $I_{\mathcal{S}}$  is the ideal of 2-minors of the matrix

$$M := \begin{bmatrix} x_1 & \dots & x_5 & y_1 & \dots & y_6 \\ x_2 & \dots & x_6 & y_2 & \dots & y_7 \end{bmatrix}.$$

The matrix  $\mathcal{A}$  providing the parametrization of the scroll is

$$\mathcal{A} = \begin{bmatrix} 1 & 1 & \dots & 1 & 1 & \dots & 1 \\ 0 & 0 & \dots & 0 & 1 & \dots & 1 \\ 1 & 2 & \dots & 6 & 1 & \dots & 7 \end{bmatrix}.$$

The number and degrees of elements in the universal Gröbner basis of the ideal  $I_{\mathcal{A}}$  can be found in the Table of degrees. The primitive colored partition identity of maximal degree is

$$1_1+1_1+1_1+1_1+1_1+1_1+7_2+7_2+7_2+7_2+7_2 = 1_2+1_2+1_2+1_2+1_2+6_1+6_1+6_1+6_1+6_1+6_1.$$

The corresponding binomial in the ideal  $I_{\mathcal{A}}$  is

$$x_1^6 y_7^5 = y_1^5 x_6^6.$$

The state polytope of the ideal  $I_{\mathcal{A}}$  is 10-dimensional.

There exist primitive elements that are not circuits. In fact, using [42], we can see that there is a circuit in every degree from 2 to 11 except degree 10, but the number of circuits in each degree is considerably smaller than the number of primitive binomials.

## Chapter 4

### Phylogenetic ideals

The contents of this chapter is drawn from the joint paper with Julia Chifman. We address the problem of studying the toric ideals of phylogenetic invariants for a general group-based model on an arbitrary claw tree. We focus on the group  $\mathbb{Z}_2$  and choose a natural recursive approach that extends to other groups. The study of the lattice associated with each phylogenetic ideal produces a list of circuits that generate the corresponding lattice basis ideal. In addition, we describe *explicitly* a quadratic lexicographic Gröbner basis of the toric ideal of invariants for the claw tree on an arbitrary number of leaves. Combined with a result of Sturmfels and Sullivant, this implies that the phylogenetic ideal of *every* tree for the group  $\mathbb{Z}_2$  has a quadratic squarefree Gröbner basis. Hence, the coordinate ring of the toric variety is Cohen-Macaulay and a Koszul algebra.

#### 4.1 Background

Phylogenetics is concerned with determining genetic relationship between species based on their DNA sequences. First, the various DNA sequences are aligned, that is, a correspondence is established that accounts for their differences. Assuming that all DNA sites evolve identically and independently, the focus is on one site at a time. The data then consists of observed pattern frequencies in aligned sequences. This observed data are used to estimate the true joint probabilities of the observations and, most importantly, to reconstruct the ancestral relationship among the species. The relationship can be represented by a phylogenetic tree.

A *phylogenetic tree*  $T$  is a simple, connected, acyclic graph equipped with some statistical information. Namely, each node of  $T$  is a random variable with  $k$  possible states chosen from the state space  $S$ . Edges of  $T$  are labeled by transition probability matrices that reflect probabilities of changes of the states from a node to its child. These probabilities of mutation are the parameters for the statistical model of evolution, which is described in terms of a discrete-state continuous-time Markov process on the tree. Since the goal is to reconstruct the tree, the interior nodes are hidden. The relationship between the random variables is encoded by the structure of the tree. At each of the  $n$  leaves, we can observe any of the  $k$  states; thus there are  $k^n$  possible observations. Let  $p_\sigma$  be the joint probability of making a particular observation  $\sigma \in S^n$  at the leaves. Then  $p_\sigma$  is a polynomial in the model parameters. A *phylogenetic invariant* of the model is a polynomial in the leaf probabilities which vanishes for every choice of model parameters. The set of these polynomials forms a prime ideal in the polynomial ring over the unknowns  $p_\sigma$ . The objective is to compute this ideal explicitly. Thus we consider a polynomial map  $\phi : \mathbb{C}^N \rightarrow \mathbb{C}^{k^n}$ , where  $N$  is the total number of model parameters. The map depends only on the

tree  $T$  and the number of states  $k$ ; its coordinate functions are the  $k^n$  polynomials  $p_\sigma$ . The map  $\phi$  induces a parametrization of an algebraic variety. The study of these algebraic varieties for various statistical models is a central theme in the field of algebraic statistics ([35]). Phylogenetic invariants are a powerful tool for tree reconstruction ([3], [9], [20]). In fact, to reconstruct the phylogenetic trees in practice, it is sufficient to have a complete intersection inside of the ideal of invariants, and not necessarily the entire toric ideal. In view of this result ([9]), the lattice basis ideal, which we compute, is a good candidate.

There is a specific class of models for which the ideal of invariants is particularly nice. Let  $M_e$  be the  $k \times k$  transition probability matrix for edge  $e$  of  $T$ . In the general Markov model, each matrix entry is an independent model parameter. A group-based model is one in which the matrices  $M_e$  are pairwise distinct, but it is required that certain entries coincide. For these models, transition matrices are diagonalizable by the Fourier transform of an abelian group. The key idea behind this linear change of coordinates is to label the states (for example,  $A, C, G$ , and  $T$ ) by a finite abelian group (for example,  $\mathbb{Z}_2 \times \mathbb{Z}_2$ ) in such a way that transition from one state to another depends only on the difference of the group elements. Examples of group-based models include the Jukes-Cantor and Kimura's one-parameter models used in computational biology.

Sturmfels and Sullivant in [35] reduce the computation of ideals of phylogenetic invariants of group-based models on an arbitrary tree to the case of claw trees  $T_n := K_{1,n}$ , the complete bipartite graph from one node (the root) to  $n$  nodes (the leaves). The main result of [35] gives a way of constructing the ideal of phylogenetic invariants for any tree *if* the ideal for the claw tree is known. However, in general, it is an open problem to compute the phylogenetic invariants for a claw tree. We consider the ideal for a general group-based model for the group  $\mathbb{Z}_2$ . Let  $q_\sigma$  be the image of  $p_\sigma$  under the Fourier transform. Assuming the identity labelling function and adopting the notation of [35], the ideal of phylogenetic invariants for the tree  $T_n$  is the kernel of the following homomorphism between polynomial rings:

$$\begin{aligned} \varphi_n : \mathbb{C}[q_{g_1, \dots, g_n} : g_1, \dots, g_n \in G] &\rightarrow \mathbb{C}[a_g^{(i)} : g \in G, i = 1, \dots, n+1] \\ q_{g_1, \dots, g_n} &\mapsto a_{g_1}^{(1)} a_{g_2}^{(2)} \dots a_{g_n}^{(n)} a_{g_1+g_2+\dots+g_n}^{(n+1)}, \end{aligned} \quad (*)$$

where  $G$  is a finite group with  $k$  elements, each corresponding to a state. The coordinate  $q_{g_1, \dots, g_n}$  corresponds to observing the element  $g_1$  at the first leaf of  $T$ ,  $g_2$  at the second, and so on. The phylogenetic invariants form a *toric ideal* in the Fourier coordinates  $q_\sigma$ , which can be computed from the corresponding lattice basis ideal by saturation. The main result of this paper is a complete description of the lattice basis ideal and a quadratic Gröbner basis of the ideal of invariants for the group  $\mathbb{Z}_2$  on  $T_n$  for any number of leaves  $n$ .

This chapter is organized as follows. In section 4.2 we lay the foundation for our recursive approach. The ideal of the two-leaf claw tree is trivial, so we begin with the case when the number of leaves is three. Sections 4.4 and 4.3 address the problem of describing the lattices corresponding to the toric ideals. We provide a nice lattice basis consisting of circuits. The corresponding lattice basis ideal is generated by cir-

cuits of degree two and thus in particular satisfies the Sturmfels-Sullivant conjecture. As described in the introductory chapter, the ideal of phylogenetic invariants is the saturation of the lattice basis ideal. However, we do not use any of the standard algorithms to compute saturation (e.g. [22], [34]). Instead, our recursive construction of the lattice basis ideals can be extended to give the full ideal of invariants, which we describe in section 4.5. The recursive description of these ideals depends only on the number of leaves of the claw tree and it does not require saturation. Finally, and possibly somewhat surprisingly, we show that the ideal of invariants for every claw tree admits a quadratic Gröbner basis with respect to a lexicographic term order. We describe it *explicitly*.

Combined with the main result of Sturmfels and Sullivant in [35], this implies that the phylogenetic ideal of *every* tree for the group  $\mathbb{Z}_2$  has a quadratic Gröbner basis. Hence, the coordinate ring of the toric variety is a Koszul algebra. In addition, the ideals for every tree can be computed explicitly. These ideals are particularly nice as they satisfy the conjecture in [35] which proposes that the order of the group gives an upper bound for the degrees of minimal generators of the ideal of invariants. The case of  $\mathbb{Z}_2$  has been solved in [35] using a technique that does not generalize. We hope to extend our recursive approach and obtain the result for an arbitrary abelian group.

For a detailed background on phylogenetic trees, invariants, group-based models, Fourier coordinates, labelling functions and more, the reader should refer to [2], [19], [29], [35]. The comprehensive background is omitted here, as the definition of the phylogenetic ideal  $\ker \varphi_n$  is sufficient for understanding this Chapter.

## 4.2 Matrix representation

Fix a claw tree  $T_n$  on  $n$  leaves and a finite abelian group  $G$  of order  $k$ . Soon we will specialize to the case  $k = 2$ . We want to compute the ideal of phylogenetic invariants for the general group-based model on  $T_n$ . After the Fourier transform, the ideal of invariants (in Fourier coordinates) is given by  $I_n = \ker \varphi_n$ , where  $\varphi_n$  is a map between polynomial rings in  $k^n$  and  $k(n+1)$  variables, respectively, defined by (\*). In order to compute the toric ideal  $I_n$ , we first compute the lattice basis ideal  $I_{L_n} \subset I_n$  corresponding to  $\varphi_n$  as follows. Fixing an order on the monomials of the two polynomial rings, the linear map  $\varphi$  can be represented by a matrix  $B_{n,k}$  that describes the action of  $\varphi$  on the variables. Then the lattice  $L_n = \ker(B_{n,k}) \subset \mathbb{Z}^{k^n}$  determines the ideal  $I_{L_n}$ . It is generated by elements of the form  $(\prod q_{g_1, \dots, g_n})^{v^+} - (\prod q_{g_1, \dots, g_n})^{v^-}$  where  $v = v^+ - v^- \in L_n$ . We will give an explicit description of this basis and, equivalently, the ideals  $I_{L_n}$ .

Hereafter assume that  $G = \mathbb{Z}_2$ . For simplicity, let us say that  $B_n := B_{n,2}$ .

To create the matrix  $B_n$ , first order the two bases as follows. Order the  $a_g^{(i)}$  by varying the upper index ( $i$ ) first and then the group element  $g$ :  $a_0^{(1)}, a_0^{(2)}, \dots, a_0^{(n+1)}, a_1^{(1)}, \dots, a_1^{(n+1)}$ . Then, order the  $q_{g_1, \dots, g_n}$  by ordering the indices with respect to binary counting:

$$q_{0\dots 00} > q_{0\dots 01} > \dots > q_{1\dots 10} > q_{1\dots 1}.$$



That is,  $q_{g_1 \dots g_n} > q_{h_1 \dots h_n}$  if and only if  $(g_1 \dots g_n)_2 < (h_1 \dots h_n)_2$ , where

$$(g_1 \dots g_n)_2 := g_1 2^{n-1} + g_2 2^{n-2} + \dots + g_n 2^0$$

represents the binary number  $g_1 \dots g_n$ .

Next, index the rows of  $B_n$  by  $a_g^{(i)}$  and its columns by  $q_{g_1, \dots, g_n}$ . Finally, put 1 in the entry of  $B_n$  in the row indexed by  $a_g^{(i)}$  and column indexed by  $q_{g_1, \dots, g_n}$  if  $a_g^{(i)}$  divides the image of  $q_{g_1, \dots, g_n}$ , and 0 otherwise.

**Example 4.2.1.** Let  $n = 2$ . Then we order the  $q_{ij}$  variables according to binary counting:  $q_{00}, q_{01}, q_{10}, q_{11}$ , so that

$$\begin{aligned} \varphi : \mathbb{C}[q_{00}, q_{01}, q_{10}, q_{11}] &\rightarrow \mathbb{C}[a_0^{(1)}, a_0^{(2)}, a_0^{(3)}, a_1^{(1)}, a_1^{(2)}, a_1^{(3)}] \\ q_{00} &\mapsto a_0^{(1)} a_0^{(2)} a_{0+0}^{(3)} \\ q_{01} &\mapsto a_0^{(1)} a_1^{(2)} a_{0+1}^{(3)} \\ q_{10} &\mapsto a_1^{(1)} a_0^{(2)} a_{1+0}^{(3)} \\ q_{11} &\mapsto a_1^{(1)} a_1^{(2)} a_{1+1}^{(3)}. \end{aligned}$$

Now we put the  $a_i^{(j)}$  variables in order:  $a_0^{(1)}, a_0^{(2)}, a_0^{(3)}, a_1^{(1)}, a_1^{(2)}, a_1^{(3)}$ . Thus

$$B_2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

The tree  $T_{n-1}$  can be considered as a subtree of  $T_n$  by ignoring, for example, the leftmost leaf of  $T$ . As a consequence, a natural question arises: how does  $B_n$  relate to  $B_{n-1}$ ?

**Remark 4.2.2.** The matrix  $B_{n-1}$  for the subtree of  $T_n$  with the leaf (1) removed can be obtained as a submatrix of  $B_n$  for the tree  $T_n$  by deleting rows 1 and  $(n+1)+1$  and taking only the first  $2^{n-1}$  columns.

Divide the  $n$ -leaf matrix  $B_n$  into a  $2 \times 2$  block matrix with blocks of size  $(n+1) \times 2^{n-1}$ :

$$B_n = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}.$$

Then, grouping together  $B_{11}, B_{21}$  without the first row of each  $B_{i1}$ , we obtain the matrix  $B_{n-1}$ . This is true because rows 1 and  $(n+1)+1$  represent the variables  $a_g^{(1)}$  for  $g \in G$  associated with the leaf (1) of  $T_n$ . Note that the entries in row  $a_g^{(n+1)}$  remain undisturbed as the omitted rows are indexed by the identity of the group.

**Example 4.2.3.** The matrix  $B_2$  is equal to the submatrix of  $B_3$  formed by rows 2,3,4,6,7,8, and first 4 columns.

**Remark 4.2.4.** Fix any observation  $\sigma = g_1, \dots, g_n$  on the leaves. Clearly, at any given leaf  $j \in \{1, \dots, n\}$ , we observe exactly one group element,  $g_j$ . Since the matrix entry  $b_{a_{g_j}^{(j)}, q_\sigma}$  in the row indexed by  $a_{g_j}^{(j)}$  and column indexed by  $q_\sigma$  is 1 exactly when  $a_{g_j}^{(j)}$  divides the image of  $q_\sigma$ , one has that

$$\sum_{g_j \in G} b_{a_{g_j}^{(j)}, q_\sigma} = 1$$

for a fixed leaf  $(j)$  and fixed observation  $\sigma$ . Note that the formula also holds if  $j = n + 1$  by definition of  $a_{g_{n+1}}^{(n+1)} = a_{g_1 + \dots + g_n}^{(n+1)}$ . In particular, the rows indexed by  $a_{g_j}^{(j)}$  for a fixed  $j$  sum up to the row of ones.

### 4.3 Number of lattice basis elements

We compute the dimension of the kernel of  $B_n$  by induction on  $n$ . We proceed in two steps.

**Lemma 4.3.1** (Lower bound).

$$\text{rank}(B_n) \geq \text{rank}(B_{n-1}) + 1.$$

*Proof.* First note that  $\text{rank}(B_n) \geq \text{rank}(B_{n-1})$  since  $B_{n-1}$  is a submatrix of the first  $2^{n-1}$  columns of  $B_n$ . In the block  $[B_{11}, B_{12}]^T$ , the row indexed by  $a_1^{(1)}$  is zero, while in the block  $[B_{21}, B_{22}]^T$ , the row indexed by  $a_1^{(1)}$  is 1. Choosing one column from  $[B_{21}, B_{22}]^T$  provides a vector independent of the first  $2^{n-1}$  columns. The rank must therefore increase by at least 1.  $\square$

**Lemma 4.3.2** (Upper bound).

$$\text{rank}(B_n) \leq n + 2.$$

*Proof.*  $B_n$  has  $2(n + 1)$  rows. Remark 4.2.4 provides  $n$  independent relations among the rows of our matrix: varying  $j$  from 1 to  $n + 1$ , we obtain that the sum of the rows  $j$  and  $n + 1 + j$  is 1 for each  $j = 1, \dots, n + 1$ . Thus the upper bound is immediate.  $\square$

We are ready for the main result of the section.

**Proposition 4.3.3** (Cardinality of lattice basis). *Let  $n \geq 2$ . Then there are  $2^n - 2(n + 1) + n$  elements in the basis of the lattice  $L_n$  corresponding to  $T_n$ . That is,*

$$\dim \ker(B_n) = 2^n - 2(n + 1) + n.$$

*Proof.* We show  $\text{rank}(B_n) = 2(n + 1) - n$ . It can be checked directly that  $B_2$  has full rank. Assume that the claim is true for  $n - 1$ . Then by Lemmata (4.3.1) and (4.3.2),

$$2(n + 1) - n \geq \text{rank}(B_n) \geq \text{rank}(B_{n-1}) + 1 = 2n - (n - 1) + 1,$$

where the last equality is provided by the induction hypothesis. The claim follows since the left- and the right-hand sides agree.  $\square$

#### 4.4 Lattice basis

In this section we describe a basis of the kernel of  $B_n := B_{n,2}$ , in which the binomials corresponding to the basis elements satisfy the conjecture on the degrees of the generators of the phylogenetic ideal. In particular, since the ideal is generated by squarefree binomials and contains no linear forms, these elements are actually circuits. By Proposition 4.3.3, we need to find  $2^n - (n + 2)$  linearly independent vectors in the lattice. The matrix of the tree with  $n = 2$  leaves has a trivial kernel, so we begin with the tree on  $n = 3$  leaves. The dimension of the kernel is 3 and the lattice basis is given by the rows of the following matrix:

$$\begin{bmatrix} 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & -1 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 \end{bmatrix}.$$

In order to study the kernels of  $B_n$  for any  $n$ , it is useful to have an algorithmic way of constructing the matrices.

**Algorithm 4.4.1.** [The construction of  $B_n$ ]

**Input:** the number of leaves  $n$  of the claw tree  $T_n$ .

**Output:**  $B_n \in \mathbb{Z}^{2(n+1) \times 2^n}$ .

Initialize  $B_n$  to the zero matrix.

Construct the first  $n$  rows:

for  $k$  from 1 to  $n$  do:

for  $c$  from 0 to  $2^k - 1$  with  $c \equiv 0 \pmod{2}$  do:

for  $j$  from  $c2^{n-k} + 1$  to  $(c + 1)2^{n-k}$  do:  $b_{k,j} := 1$ .

Construct row  $n + 1$ :

if  $n \equiv (\sum_{r=1}^n b_{r,j}) \pmod{2}$ , then  $b_{n+1,j} := 1$ .

Construct rows  $n + 2$  to  $2(n + 1)$ :

for  $i$  from 1 to  $n + 1$  do:

for  $j$  from 1 to  $2^n$  do:  $b_{n+1+i,j} := 1 - b_{i,j}$ .

One checks that this algorithm gives indeed the matrices  $B_n$  as defined in Section 4.2.

The  $(n + 1 + i)^{th}$  row  $r_{n+1+i}$  of  $B_n$  is by definition the binary complement of the  $i^{th}$  row  $r_i$  of  $B_n$ . Suppose that  $r_i \cdot k = 0$  for some vector  $k$ . Since all entries of  $B_n$  are nonnegative, a subvector of  $k$  restricted to the entries where  $r_i$  is nonzero must be homogeneous in the sense that the sum of the positive entries equals the sum of the negative entries. But since the ideal  $I_{L_n}$  itself is homogeneous ([34]), the same must be true for the subvector of  $k$  restricted to the entries where  $r_i$  is zero. Hence  $r_{n+1+i} \cdot k = 0$ . Therefore, it is enough to analyze the top half of the matrix  $B_n$  when determining the kernel elements.

**Remark 4.4.2.** There are  $n$  copies of  $B_{n-1}$  inside  $B_n$ .

By deleting one leaf at a time, we get  $n$  copies of  $T_{n-1}$  as a subtree of  $T_n$ . Suppose we delete leaf  $(i)$  from  $T_n$  to get the tree  $T_n^{(i)}$  on leaves  $1, 2, \dots, i-1, i+1, \dots, n$ . Ignoring the two rows of  $B_n$  that represent the leaf  $(i)$  and taking into account the columns

of  $B_n$  containing nonzero entries of the row indexed by  $a_0^{(i)}$  (that is, observing 0 at leaf  $(i)$ ) gives precisely the matrix  $B_{n-1}$  corresponding to  $T_n^{(i)}$ . Note that the entry indexed by  $a_g^{(n+1)}$ , for any  $g \in G$ , will be correct since we are ignoring the identity of the group, as in Remark 4.2.2.

This leads to a way of constructing a basis of  $\ker(B_n)$  from the one of  $\ker(B_{n-1})$ . Namely, removing leaf (1) from  $T_n$  produces  $\dim(\ker(B_{n-1})) = 2^{n-1} - n - 1$  independent vectors in  $\ker(B_n)$ . Let us name this collection of vectors  $V_1$ . Removing leaf (2) produces a collection  $V_2$  consisting of  $\dim(\ker B_{n-1}) - \dim(\ker B_{n-2}) = 2^{n-2} - 1$  vectors in  $\ker(B_n)$ .  $V_2$  is independent of  $V_1$  since the second half of each vector in  $V_2$  has nonzero entries in the columns of  $B_n$  where all vectors in  $V_1$  are zero, a direct consequence of the location of the submatrix corresponding to  $T_n^{(2)}$ . Finally, removing any other leaf  $(i)$  of  $T_n$  produces a collection  $V_i$  of as many new kernel elements as there are new columns involved (in terms of the submatrix structure); namely,  $2^{n-i}$  new vectors. Note that every vector in  $V_2$  has a nonzero entry in at least one new column so that the full collection is independent of  $V_1$ .

Using the above procedure, we have obtained

$$(2^{n-1} - n - 1) + (2^{n-2} - 1) + (2^{n-3}) + \dots + 2^{n-n}$$

independent vectors in the kernel of  $B_n$ . This is exactly one less than the desired number,  $2^n - n - 2$ . Hence to the list of the kernel generators we add one additional vector  $v$  that is independent of all the  $V_i$ ,  $i = 1, \dots, n$  as it has a nonnegative entry in the last column. (Note that no  $v \in V_i$  has this property by the observation on the column location of the submatrix associated with each  $T_n^{(i)}$ .) In particular,  $v = [0, \dots, 0, 1, 0, 0, -1, -1, 0, 0, 1] \in \ker(B_n)$ . To see this, we simply notice that the rows of the last 8-column block of  $B_n$  are precisely the rows of the first 8-column block of  $B_n$  up to permutation of rows, which does not affect the kernel.

The lattice basis we just constructed is directly computed by the following algorithm.

**Algorithm 4.4.3.** [Construction of the lattice basis for  $T_n$ ]

**Input:** the number of leaves  $n$  of the claw tree  $T_n$ .

**Output:** a basis of  $\ker B_n$  in form of a  $(2^n - n - 2) \times 2^n$  matrix  $L_n$ .

$$\text{Let } L_3 := \begin{bmatrix} 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & -1 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 \end{bmatrix}.$$

Set  $k := 4$ .

The following subroutine lifts  $L_{k-1}$  to  $L_k$ :

WHILE  $k \leq n$  do: {

Initialize  $L_k$  to the zero matrix.

For  $i$  from 1 to  $k$  do:

$$\text{cols}(i) := \{1..2^{k-i}, (2)2^{k-i} + 1..(3)2^{k-i}, \dots, (2^i - 2)2^{k-i} + 1..(2^i - 1)2^{k-i}\}.$$

Denote by  $L_{k,j}[\text{cols}(i)]$  the  $j^{\text{th}}$  row vector of  $L_k$  restricted to columns  $\text{cols}(i)$ .

Set  $i := 1$ :

$$\text{for } j \text{ from } 1 \text{ to } 2^{k-1} - k - 1 \text{ do: } L_{k,j}[\text{cols}(i)] := L_{k-1,j}.$$

Set  $i := 2$ :

for  $j$  from 1 to  $2^{k-2} - 1$  do :  
 $L_{k,(2^{k-1}-k-1)+j}[\text{cols}(i)] := L_{k-1,(2^{k-1}-k-1)-(2^{k-2}-1)+j}$ .  
 For  $i$  from 3 to  $k$  do:  
 for  $j$  from 1 to  $2^{k-i}$  do:  
 $L_{k,(2^k-2^{k+1-i}-k-2)+j}[\text{cols}(i)] := L_{k-1,(2^{k-1}-k-1)-(2^{k-i})+j}$ .  
 Finally,  $L_{k,2^k-k-2}[2^k - 7..2^k] := [1, 0, 0, -1, -1, 0, 0, 1]$ .  
 RETURN  $L_k$ . }

**Example 4.4.4.** Consider the tree on  $n = 4$  leaves. Then

$$B_4 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

The lattice basis is given by the rows of the following matrix:

$$L_4 = \begin{bmatrix} 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & -1 & 0 & 0 \end{bmatrix}.$$

The lattice vectors correspond to the relations on the leaf observations in the natural way; namely, the first column corresponds to  $q_{0,\dots,0}$ , the second to  $q_{0,\dots,0,1}$ , and so on.

Therefore, the lattice basis ideal for  $T_4$  in Fourier coordinates is

$$I_{L_4} = (q_{0010}q_{0101} - q_{0011}q_{0100}, q_{0001}q_{0110} - q_{0011}q_{0100}, q_{0000}q_{0111} - q_{0011}q_{0100}, \\ q_{0010}q_{1001} - q_{0011}q_{1000}, q_{0001}q_{1010} - q_{0011}q_{1000}, q_{0000}q_{1011} - q_{0011}q_{1000}, \\ q_{0001}q_{1100} - q_{0101}q_{1000}, q_{0000}q_{1101} - q_{0101}q_{1000}, \\ q_{0000}q_{1110} - q_{0110}q_{1000}, q_{1000}q_{1111} - q_{1011}q_{1100}).$$

This ideal is contained in the ideal of phylogenetic invariants  $I_4$  for  $T_4$ .

As mentioned earlier, the lattice basis ideal is a good candidate for a complete intersection ideal inside the ideal of invariants for any  $n$ . In [9] it was shown that in order to use invariants for phylogenetic inference, one only needs to consider a local complete intersection at the interesting points. Therefore the lattice basis we provide could be used for phylogenetic reconstruction once we show it is indeed a complete intersection containing the phylogenetic variety. Then, our complete intersection will define the variety at most of the points because of Corollary 2.1 in [25].

To prove that the lattice basis ideal defines a complete intersection, we simply use the criterion given in Theorem 2.1. in [10]. The criterion requires that the matrices  $B_n$  have the following property: each submatrix  $B'_n$  of  $B_n$  such that every row has a positive and a negative entry must have at least as many columns as there are rows. But by our recursive construction of the lattice bases  $B_n$ , the pattern of 1's and  $-1$ 's widens as we add more rows to the matrix. If we choose a 1-row submatrix  $B'_n$ , there must be 2 columns thus the criterion is trivially satisfied. Suppose we wish to add one more row to  $B'_n$ : then we must add at least one more column by the construction of the row pattern of  $B_n$ . The only time we might not add another column is when choosing a submatrix  $B'_n$  with two identical rows, which is the irrelevant case. We thus conclude that the complete intersection criterion is satisfied for all  $B_n$ .

## 4.5 Ideal of invariants

In this section, we compute explicitly all of the generators of the ideal of invariants for any claw tree  $T_n$  and the group  $\mathbb{Z}_2$ . We show that the lattice basis ideals provide basic building blocks for the full ideals of invariants, as expected. However, instead of computing the ideal of invariants as a saturation of the lattice basis ideal in a standard way (e.g. [22],[34]), we use the recursive constructions from the previous section on the saturated ideals directly. We begin with the ideal of invariants for the smallest tree, and build all other trees recursively. The underlying ideas for how to lift the generating sets come from Algorithm 4.4.3.

We will denote the ideal of the claw tree on  $n$  leaves by  $I_n = \ker \varphi_n$ . As we have seen, the first nontrivial ideal is  $I_3$ .

### 4.5.1 The tree on 3 leaves

**Claim 4.5.1.** *The ideal of the claw tree on  $n = 3$  leaves is*

$$I_3 = (q_{000}q_{111} - q_{100}q_{011}, q_{001}q_{110} - q_{100}q_{011}, q_{010}q_{101} - q_{100}q_{011}).$$

This can be verified by computation. In particular, this ideal is equal to the lattice basis ideal for the tree on three leaves;  $I_{L_3}$  is already prime in this case. Let  $< := <_{lex}$  be the lexicographic order on the variables induced by

$$q_{000} > q_{001} > q_{010} > q_{011} > q_{100} > q_{101} > q_{110} > q_{111}.$$

(That is,  $q_{ijk} > q_{i'j'k'}$  if and only if  $(ijk)_2 < (i'j'k')_2$ , where  $(ijk)_2$  denotes the binary number  $ijk$ .)

**Remark 4.5.2.** The three generators of  $I_3$  above are a Gröbner basis for  $I_3$  with respect to  $<$ , since the initial terms, written with coefficient +1 in the above description, are relatively prime so all the S-pairs reduce to zero.

**Remark 4.5.3.** Write the quadratic binomial  $q = q^+ - q^-$  as

$$q_{g_1^{(1)}g_1^{(2)}g_1^{(3)}}q_{g_2^{(1)}g_2^{(2)}g_2^{(3)}} - q_{h_1^{(1)}h_1^{(2)}h_1^{(3)}}q_{h_2^{(1)}h_2^{(2)}h_2^{(3)}}.$$

Then  $q \in I_3$  if and only if the following two conditions hold:

1. Exchanging the roles of  $q_{h_1^{(1)}h_1^{(2)}h_1^{(3)}}$  and  $q_{h_2^{(1)}h_2^{(2)}h_2^{(3)}}$  if necessary,

$$g_1^{(1)} + g_1^{(2)} + g_1^{(3)} = h_1^{(1)} + h_1^{(2)} + h_1^{(3)}$$

and

$$g_2^{(1)} + g_2^{(2)} + g_2^{(3)} = h_2^{(1)} + h_2^{(2)} + h_2^{(3)},$$

2.  $g_1^{(i)} + g_2^{(i)} = 1 = h_1^{(i)} + h_2^{(i)}$  for  $1 \leq i \leq 3 = n$ .

Note that the second condition holds since otherwise the projection of  $q$  obtained by eliminating the leaf  $(i)$  at which the observations  $g_1^{(i)}$  and  $g_2^{(i)}$  are both equal to 0 or to 1 produces an element  $q'$  in the kernel of the map  $\varphi_2$  of the 2-leaf tree, which is trivial.

#### 4.5.2 The tree on an arbitrary number of leaves

Let us now define a set of maps and a distinguished set of binomials in  $I_n$ .

**Definition 4.5.4.** Let  $\pi_i(q)$  be the projection of  $q$  that eliminates the  $i^{th}$  index of each variable in  $q$ .

For example,

$$\pi_4(q_{0000}q_{1110} - q_{1000}q_{0110}) = q_{000}q_{111} - q_{100}q_{011}.$$

**Definition 4.5.5.** Assume that  $n \geq 4$ .

Let  $\mathcal{G}_n$  be the set of quadratic binomials  $q \in I_n$  that can be written as

$$q = q^+ - q^- = q_{g_1^{(1)} \dots g_1^{(n)}}q_{g_2^{(1)} \dots g_2^{(n)}} - q_{h_1^{(1)} \dots h_1^{(n)}}q_{h_2^{(1)} \dots h_2^{(n)}}$$

such that one of the two following properties is satisfied:

Property (i): For *some*  $1 \leq i \leq n$ ,  $j \in \mathbb{Z}_2$ ,

$$g_1^{(i)} = g_2^{(i)} = j = h_1^{(i)} = h_2^{(i)} \quad (4.1)$$

and

$$\pi_i(q) \in I_{n-1}. \quad (4.2)$$

Property (ii): For *each*  $1 \leq k \leq n$ ,

$$g_1^{(k)} + g_2^{(k)} = 1 = h_1^{(k)} + h_2^{(k)} \quad (4.3)$$

and

$$\pi_k(q) \in I_{n-1}. \quad (4.4)$$

**Example 4.5.6.** Let  $n = 4$ . The set of elements  $q \in \mathcal{G}_n$  with Property (i) consists of those for which  $j = 0$ :

$q_{0000}q_{0111} - q_{0100}q_{0011}$ ,  $q_{0001}q_{0110} - q_{0100}q_{0011}$ ,  $q_{0010}q_{0101} - q_{0100}q_{0011}$ ,  
 $q_{0000}q_{1011} - q_{1000}q_{0011}$ ,  $q_{0001}q_{1010} - q_{1000}q_{0011}$ ,  $q_{0010}q_{1001} - q_{1000}q_{0011}$ ,  
 $q_{0000}q_{1101} - q_{1000}q_{0101}$ ,  $q_{0001}q_{1100} - q_{1000}q_{0101}$ ,  $q_{0100}q_{1001} - q_{1000}q_{0101}$ ,  
 $q_{0000}q_{1110} - q_{1000}q_{0110}$ ,  $q_{0010}q_{1100} - q_{1000}q_{0110}$ ,  $q_{0100}q_{1010} - q_{1000}q_{0110}$ ;  
and those for which  $j = 1$ :

$q_{1000}q_{1111} - q_{1100}q_{1011}$ ,  $q_{1001}q_{1110} - q_{1100}q_{1011}$ ,  $q_{1010}q_{1101} - q_{1100}q_{1011}$ ,  
 $q_{0100}q_{1111} - q_{1100}q_{0111}$ ,  $q_{0101}q_{1110} - q_{1100}q_{0111}$ ,  $q_{0110}q_{1101} - q_{1100}q_{0111}$ ,  
 $q_{0010}q_{1111} - q_{1010}q_{0111}$ ,  $q_{0011}q_{1110} - q_{1010}q_{0111}$ ,  $q_{0110}q_{1011} - q_{1010}q_{0111}$ ,  
 $q_{0001}q_{1111} - q_{1001}q_{0111}$ ,  $q_{0011}q_{1101} - q_{1001}q_{0111}$ ,  $q_{0101}q_{1011} - q_{1001}q_{0111}$ .

The set of elements  $q \in \mathcal{G}_n$  with Property (ii) are:

$q_{0000}q_{1111} - q_{1001}q_{0110}$ ,  $q_{0001}q_{1110} - q_{1000}q_{0111}$ ,  $q_{0011}q_{1100} - q_{1001}q_{0110}$ ,  
 $q_{0010}q_{1101} - q_{1000}q_{0111}$ ,  $q_{0101}q_{1010} - q_{1001}q_{0110}$ ,  $q_{0100}q_{1011} - q_{1000}q_{0111}$ .

**Proposition 4.5.7.** For  $n \geq 4$ , the set of binomials in  $\mathcal{G}_n$  generates the ideal  $I_n$ . That is,

$$I_n = (q : q^+ - q^- \in \mathcal{G}_n).$$

In addition, this set of generators can be obtained inductively by lifting the generators corresponding to the various phylogenetic ideals on  $n - 1$  leaves.

*Proof.* Condition (4.3) is simply the negation of (4.1). Condition (4.1) can be restated as follows: for some  $1 \leq i \leq n$  and a fixed  $j$ ,

$$(a_j^{(i)})^2 | \varphi_n(q^+) \text{ and } (a_j^{(i)})^2 | \varphi_n(q^-).$$

Therefore, Property (i) translates to having an observation  $j$  fixed at leaf  $(i)$  for each of the variables in  $q$ . On the other hand, condition (4.3) means that for any  $k$ , not all the  $k^{\text{th}}$  indices are 0 and not all are 1. Thus Property (ii) means that no leaf has a fixed observation, and can be restated as follows: for every  $1 \leq i \leq n$ ,

$$a_0^{(i)} a_1^{(i)} | \varphi_n(q^+) \text{ and } a_0^{(i)} a_1^{(i)} | \varphi_n(q^-). \quad (4.5)$$



By definition, the ideal  $I_n$  is toric, so it is generated by binomials. In fact, it is generated by homogeneous binomials, because each row of the matrix  $B_n$  used for defining it has row sum  $n+1$  ([34], chapter 4). In addition, Sturmfels and Sullivant in [35] have shown that the ideal  $I_n$  is generated in degree 2. Hence it suffices to consider homogeneous quadratic binomials. Let  $q = q^+ - q^-$  be a binomial in  $I_n$  of degree 2. Then clearly either (4.1) or (4.3) holds; that is, either the index corresponding to one leaf is fixed for all the monomials in  $q$ , or none of them are.

In the former case, for the index  $i$  from equation (4.1),

$$\begin{aligned} q \in I_n &\iff \varphi_n(q^+) = \varphi_n(q^-) \\ &\iff \varphi_{n-1}(\pi_i(q^+)) = \varphi_{n-1}(\pi_i(q^-)) \iff \pi_i(q) \in I_{n-1}, \end{aligned}$$

where the first statement holds by definition of  $\varphi_n$  and the second by definition of the projection  $\pi_i$ .

In the latter case, for each  $i$  with  $1 \leq i \leq n$ ,

$$\begin{aligned} q \in I_n &\iff \varphi_n(q^+) = \varphi_n(q^-) \\ &\iff \varphi_{n-1}(\pi_i(q^+)) = \varphi_{n-1}(\pi_i(q^-)) \iff \pi_i(q) \in I_{n-1}, \end{aligned}$$

where the second statement holds by definition of  $\pi_i$  and (4.5). It follows that  $I_n = (q : q \in \mathcal{G}_n)$ .

In particular, the set of generators for  $I_n$  with Property (i) can be obtained from those of  $I_{n-1}$  by inserting first 0 at the  $i^{\text{th}}$  index position for each monomial of  $q \in \mathcal{G}_{n-1}$  and then repeating the same process by inserting 1. This operation corresponds to lifting to all the possible preimages of  $\pi_i(q)$  that satisfy Property (i) for each  $1 \leq i \leq n$  and every  $q \in \mathcal{G}_{n-1}$ . The set of generators for  $I_n$  with Property (ii) can be obtained from those of  $I_{n-1}$  by a similar lifting to all preimages of  $\pi_i(q)$  for each  $q \in \mathcal{G}_{n-1}$  in such a way that Property (ii) is satisfied. Namely, for every  $q = q^+ - q^- \in \mathcal{G}_{n-1}$  with Property (ii), one inserts 0 at the  $i^{\text{th}}$  index position for one monomial of  $q^+$  and for one monomial of  $q^-$ , and inserts 1 at the  $i^{\text{th}}$  index position for the remaining monomials of  $q^+$  and  $q^-$ . In addition, by definition of Property (ii), it suffices to lift to the preimages of  $\pi_n(q)$  only.  $\square$

Recall from Chapter 2 that a binomial  $q = q^+ - q^- \in I$  is said to be *primitive* if there exists no binomial  $f = f^+ - f^- \in I$  with the property that  $f^+ | q^+$  and  $f^- | q^-$ . A *circuit* is a primitive binomial of minimal support.

**Remark 4.5.8.** The binomials in  $\mathcal{G}_n$  are circuits of  $I_n$ , since the ideal is generated by squarefree binomials and contains no linear forms.

In general, we can describe the generators of  $I_n$  as follows: given  $n$ , begin by lifting  $\mathcal{G}_3$  recursively to produce  $\mathcal{G}_{n-1}$ ; that is, until the number of indices of each generator reaches  $n-1$ . Next, lift  $\mathcal{G}_{n-1}$   $n$  times so that Property (i) is satisfied for one of the  $n$  index positions. For example,

$$q := q_0000q_{1111} - q_{1001}q_{0110} \in \mathcal{G}_4$$

can be lifted to a generator of  $I_5$  in ten different ways: by lifting to preimages of  $\pi_1, \dots, \pi_5$  so that Property (i) is satisfied with either a 0 or a 1:

$$\begin{aligned}\pi_1^{-1}(q) &= \{q_{00000}q_{01111} - q_{01001}q_{00110}, q_{10000}q_{11111} - q_{11001}q_{10110}\}, \\ \pi_2^{-1}(q) &= \{q_{00000}q_{10111} - q_{10001}q_{00110}, q_{01000}q_{11111} - q_{11001}q_{01110}\},\end{aligned}$$

and so on. This will be the set of binomials in  $\mathcal{G}_n$  with Property (i). Clearly, some generators will repeat during the recursive lifting: lifting by inserting 0 at position ( $i$ ) allows the 0 to occur at the previous  $i - 1$  positions. Also, fixing 1 at any leaf allows 0 to appear on any of the other leaves.

To construct  $q^+ - q^-$  with Property (ii), we need not proceed inductively, as all projections of binomials that satisfy this property must satisfy it, too. Instead, we consider two cases corresponding to the parity of  $n$ . Namely, recalling the definition of Property (ii), first we fix  $q^-$  in such a way to ensure that  $in_{<lex}(q) = q^+$ . Suppose  $n$  is odd. Fix  $q^-$  by taking

$$q^- = q_{01\dots 1}q_{10\dots 0}$$

with  $n$  indices in each of the two variables. Then  $n - 1$  being even provides that  $a_0^{(n+1)}a_1^{(n+1)}|\varphi_n(q^-)$ . Thus every choice of  $q^+$  must satisfy the same. To find  $q^+$ , we need to choose pairs of  $n$ -digit binary numbers with digits complementary to each other, and thus there are  $2^{n-1} - 1$  choices for  $q^+$ . Specifically, listing the smallest  $2^{n-1} - 1$   $n$ -digit binary numbers and pairing them with the largest  $2^{n-1} - 1$   $n$ -digit binary numbers in reverse order produces all choices for  $q^+$ , and we have a complete list of generators. For example, the first such generator in the list would be  $q_{0\dots 0}q_{1\dots 1} - q_{01\dots 1}q_{10\dots 0}$ .

If  $n$  is even, then we can create  $q^-$  such that  $(a_0^{(n+1)})^2$  or  $(a_1^{(n+1)})^2$  divides  $\varphi_n(q^-)$  and  $\varphi_n(q^+)$ . Namely, the two choices for  $q^-$  are

$$q^- = q_{01\dots 1}q_{10\dots 0} \text{ and } q^- = q_{01\dots 10}q_{10\dots 01}.$$

The list of all possible  $q^+$  is obtained in the manner similar to the case when  $n$  is odd, except that the odd pairs in the list receive the first choice of  $q^-$ , while the even pairs receive the second. The number of such generators  $q^+ - q^-$  is  $2^{n-1} - 2$ , since there are  $2^n$   $n$ -digit binary numbers and thus half as many pairs, and 2 choices are taken by the  $q^-$ .

Next we strengthen Proposition (4.5.7).

**Proposition 4.5.9.** *The set  $\mathcal{G}_n$  is a lexicographic Gröbner basis of  $I_n$ , for any  $n \geq 4$ .*

*Proof.* For the case  $n = 3$  this is already shown. Let  $n > 3$ . Then we can partition the set of  $q \in \mathcal{G}_n$  into those satisfying Property (i) or (ii). Note that  $I_n$  is prime by definition, and thus radical. Also, Proposition (4.5.7) shows it is generated by squarefree quadratic binomials. These facts are used in what follows.

Let  $q_i, q_j \in I_n$ . If  $(q_i^+, q_j^+) = 1$ , the S-pair  $S(q_i, q_j)$  reduces to zero. Also, if  $q_i^-$  and  $q_j^-$

are not relatively prime, the cancellation criterion provides that the corresponding S-pair also reduces to zero. Therefore we consider  $f := S(q_i, q_j) \in I_n$  with  $(q_i^+, q_j^+) \neq 1$  and  $(q_i^-, q_j^-) = 1$ . In particular,  $\deg(f) = 3$ . Let us write  $q_i = q_{g_1}q_{g_2} - q_{h_1}q_{h_2}$  and  $q_j = q_{g_1}q_{g_3} - q_{h_3}q_{h_4}$ . Then

$$f = q_{g_3}q_{h_1}q_{h_2} - q_{g_2}q_{h_3}q_{h_4} \in I_n.$$

*Case I.* Suppose  $q_i$  satisfies Property (i) and  $q_j$  satisfies Property (ii). Then there exists a  $k$  such that  $\pi_k(q_i) \in I_{n-1}$ . Furthermore, Property (ii) implies that  $\pi_k(q_j) \in I_{n-1}$ . A very technical argument shows that

$$\pi_k(f) \in I_{n-1}$$

and furthermore, this projection preserves the initial terms. In summary, to check that  $\pi_k(f) \in I_{n-1}$ , it suffices to ensure that  $a_s^{(n)} | \varphi_{n-1}(\pi_k(q_{g_3}q_{h_1}q_{h_2}))$  if and only if  $a_s^{(n)} | \varphi_{n-1}(\pi_k(q_{g_2}q_{h_3}q_{h_4}))$ , where  $s$  is the sum of the observations on the leaves of the  $(n-1)$ -leaf tree obtained from  $T$  by deleting leaf  $(k)$ . There are two cases corresponding to the parity of  $n$ . If  $n$  is odd, there are additional subcases determined by the correspondence of the images of the variables in the two monomials of  $f$  under  $\varphi_{n-1}$ . The facts that  $q_i$  and  $q_j$  satisfy Properties (i) and (ii), respectively, play a crucial role in the argument. Checking all the cases then shows that  $\pi_k(f) \in I_{n-1}$  and that initial terms are preserved under this projection. Applying the induction hypothesis then finishes the proof.

*Case II.* Suppose both  $q_i$  and  $q_j$  satisfy Property (i). Then there is a  $q_k \in \mathcal{G}_n$  satisfying Property (ii) where both  $S(q_i, q_k)$  and  $S(q_j, q_k)$  reduce to zero. The three-pair criterion ([22]) provides the desired result.

*Case III.* If both  $q_i$  and  $q_j$  satisfy Property (ii), then it can be seen from the construction preceding this Proposition that the initial terms are relatively prime, so their S-polynomial need not be considered.  $\square$

Proposition 4.5.9 has important theoretical consequences. An ideal  $I \subset S$  is said to be quadratic if it is generated by quadrics.  $S/I$  is *quadratic* if its defining ideal  $I$  is quadratic, and it is *G-quadratic* if  $I$  has a quadratic Gröbner basis. It is known (e.g. [13]) that if  $S/I$  is G-quadratic, then it is Koszul (see Chapter 2), which in turn implies it is quadratic. The reverse implications do not hold in general. We have just found an infinite family of toric varieties whose coordinate rings  $S/I$  are G-quadratic.

**Corollary 4.5.10.** *The coordinate ring of the toric variety whose defining ideal is  $I_n$  is Koszul for every  $n$ .*

Moreover, we see from the construction of  $\mathcal{G}_n$  that the ideals  $I_n$  have lexicographic initial ideals which are squarefree. Therefore we have another powerful consequence:

**Corollary 4.5.11.** *The toric variety whose defining ideal is  $I_n$  is arithmetically Cohen-Macaulay for every  $n$ .*

The approach developed here produces the list of generators for the kernel of  $B_n$  all of which are of degree two. In addition, by constructing the toric ideals of invariants inductively, we are able to explicitly calculate the quadratic Gröbner bases. In light of the conjecture posed in [35] that the ideal of phylogenetic invariants for the group of order  $k$  is generated in degree at most  $k$ , we are working on generalizing the above approach to any abelian group of order  $k$ . In particular, we want to give a description of the lattice basis ideal  $I_{L_n}$  and the ideal of invariants  $I$  for  $G = \mathbb{Z}_2 \times \mathbb{Z}_2$  with generators of degree at most 4. These phylogenetic ideals are of interest to computational biologists.

## Chapter 5

### Cut ideals

Phylogenetic ideals of claw trees from Chapter 4 can be studied in the natural context of a more general class of ideals, which are described next. The contents of this chapter is drawn from joint work with Uwe Nagel.

#### 5.1 Background

Let  $G$  be any finite graph. In [36] Sturmfels and Sullivant associate a projective variety  $X_G$  to  $G$  as follows. Let  $A|B$  be an unordered partition of the vertex set of  $G$ . Each such partition defines a cut of the graph, denoted by  $Cut(A|B)$ , which is the set of edges  $\{i, j\}$  such that  $i \in A, j \in B$  or  $j \in A, i \in B$ . For each  $A|B$ , we can then assign variables to the edges according to whether they are in  $Cut(A|B)$  or not. The coordinates  $q_{A|B}$  are indexed by the unordered partitions  $A|B$ , and the variables encoding whether the edge is in the cut are  $s_{ij}$  and  $t_{ij}$  (for "separated" and "together"). The variety  $X_G$  is specified by the following homomorphism between polynomial rings:

$$\begin{aligned} \phi_G : K[q_{A|B} : A|B \text{ partition}] &\rightarrow K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } G], \\ q_{A|B} &\mapsto \prod_{\{i,j\} \in Cut(A|B)} s_{ij} \prod_{\{i,j\} \in E(G) \setminus Cut(A|B)} t_{ij} \end{aligned}$$

The cut ideal  $I_G$  is the kernel of the map  $\phi_G$ . It is a homogeneous toric ideal, since that  $\deg \phi_G(q_{A|B}) = |E(G)|$ . The variety  $X_G$  is defined by the cut ideal  $I_G$ ; we will call  $X_G$  the *cut variety* of the graph  $G$ .

If  $G$  is a clique sum of graphs  $G_1$  and  $G_2$  (i.e.,  $V(G_1) \cap V(G_2)$  is a clique of both graphs), then the ideal generators for  $I_G$  can be obtained from those of  $I_{G_1}$  and  $I_{G_2}$ , provided the size of the clique is at most 3. This is done using the operations Lift and Quad, as defined in [36]. They relate the graph-theoretic operation of clique sum to the algebraic operation of toric fiber product [40]. Their main result is Theorem 5.2.1. It provides a powerful tool for building the cut ideals of complicated graphs. Thus, we begin by investigating special graphs, namely cycles and trees. We also complement the results about  $k$ -sums by studying the cut ideal of a disjoint union (Section 5.5). However, the algebraic properties of cut ideals remain unknown in general. It is clear that the properties of the cut ideal depend on the combinatorics of the graph. Sturmfels and Sullivant pose several conjectures in this direction.

**Conjecture 5.1.1** ([36], Conjecture 3.5.). *The cut ideal  $I_G$  is generated by quadrics if and only if  $G$  is free of  $K_4$  minors (that is,  $G$  is a simple series-parallel graph).*

**Conjecture 5.1.2** ([36], Conjecture 3.7.). *The semigroup algebra  $K[q]/I_G$  is normal if and only if  $K[q]/I_G$  is Cohen-Macaulay if and only if  $G$  is free of  $K_5$  minors.*

There isn't a clear conjecture yet characterizing those  $K_5$ -free graphs that are Gorenstein.

## 5.2 Clique sums, Segre products, Gröbner bases

We recall some concepts and results that we use later on. At the end we establish a curious consequence illustrating the fact that cut ideals have quite particular properties.

Throughout, all graphs are assumed to be finite and simple. The vertex and the edge set of such a graph  $G$  are denoted by  $V(G)$  and  $E(G)$ , respectively. A *clique* of  $G$  is a subset of  $V(G)$  such that the vertex-induced subgraph of  $G$  is complete, that is, there is an edge between any two vertices. Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two graphs such that  $V_1 \cap V_2$  is a clique of both graphs. Then the *clique sum* of  $G_1$  and  $G_2$  is the graph  $G = G_1 \# G_2$  with vertex set  $V_1 \cup V_2$  and edge set  $E_1 \cup E_2$ . If the clique  $V_1 \cap V_2$  consists of  $k + 1$  vertices, then  $G$  is also called the *k-sum* of  $G_1$  and  $G_2$ . If  $0 \leq k \leq 2$ , then Sturmfels and Sullivant [36] relate the graph-theoretic operation of forming clique sums to the algebraic operation of taking toric fiber products as defined in [40]. Defining two operations, Lift and Quad, they show that the generators of the cut ideal  $I_G$  can be obtained from the generators of the cut ideals  $I_{G_1}$  and  $I_{G_2}$ . More precisely, their result is:

**Theorem 5.2.1** ([36], Theorem 2.1). *Let  $G$  be a  $k$ -sum of  $G_1$  and  $G_2$  with  $0 \leq k \leq 2$ . Denote by  $\mathbf{F}_1$  and  $\mathbf{F}_2$  binomial generating sets for the smaller cut ideals  $I_{G_1}$  and  $I_{G_2}$ . Then*

$$\mathbf{M} = \text{Lift}(\mathbf{F}_1) \cup \text{Lift}(\mathbf{F}_2) \cup \text{Quad}(\mathbf{G}_1, \mathbf{G}_2)$$

*is a generating set for the cut ideal  $I_G$ . Furthermore, if  $\mathbf{F}_1$  and  $\mathbf{F}_2$  are Gröbner bases, then there exists a term order such that  $\mathbf{M}$  is a Gröbner basis of  $I_G$ .*

Let  $X \subset \mathbb{P}^n$  be a projective subvariety over a field  $K$ . We denote its homogeneous coordinate ring by  $A_X$ . It is a standard graded  $K$ -algebra. The variety  $X$  is said to be arithmetically Cohen-Macaulay if  $A_X$  is a Cohen-Macaulay ring. The Hilbert function of  $X$  or  $A_X$  is defined by  $h_X(j) = h_{A_X}(j) = \dim_K[A_X]_j$ . If  $j \gg 0$ , then it becomes polynomial in  $j$ . This polynomial is the Hilbert polynomial  $p_X = p_{A_X}$  of  $X$  or  $A_X$ . Following [1], we define:

**Definition 5.2.2.** The variety  $X$  (or its coordinate ring  $A_X$ ) is said to be *Hilbertian* if its Hilbert function is polynomial in every non-negative degree, i.e., for every integer  $j \geq 0$ ,  $h_X(j) = p_X(j)$ .

The cut ideal of a graph  $G$  on  $n$  vertices defines a projective variety  $X_G \subset \mathbb{P}^{2^n - 1}$ . If  $G$  is the 0-sum of  $G_1$  and  $G_2$ , then its cut variety  $X_G$  is isomorphic to the Segre product of  $X_{G_1} \times X_{G_2}$ . Algebraically, this means that the coordinate ring  $A_{X_G}$  is the Segre product  $A_{X_{G_1}} \boxtimes A_{X_{G_2}}$  of  $A_{X_{G_1}}$  and  $A_{X_{G_2}}$ . The Segre product of Cohen-Macaulay rings is often not Cohen-Macaulay. The precise result is (see, e.g., [39], Theorem I.4.6):

**Lemma 5.2.3.** *Let  $A, B$  be two graded Cohen-Macaulay  $K$ -algebras that both have dimension at least two. Then their Segre product  $A \boxtimes B$  is Cohen-Macaulay if and only if  $A$  and  $B$  are Hilbertian.*

Cut ideals are examples of toric ideals by definition. Combining the above facts with Lemma 2.2.11, we obtain a somewhat surprising consequence.

**Proposition 5.2.4.** *Let  $X \subset \mathbb{P}^n$  be a toric variety of dimension at least 1. If  $I_X$  has a squarefree initial ideal, then  $X$  is Hilbertian.*

*Proof.* Theorem 5.2.1 is proved by expressing the cut ideal of a  $k$ -sum of  $I_{G_1}$  and  $I_{G_2}$  as a toric fiber product of  $I_{G_1}$  and  $I_{G_2}$ . The toric fiber product ([40]) can be defined for any two toric ideals  $I_1$  and  $I_2$ . The operations Lift and Quad are applied to the Gröbner bases  $\mathbf{F}_1$  and  $\mathbf{F}_2$  of the ideals  $I_1$  and  $I_2$ , respectively, to provide a Gröbner basis of the toric fiber product. As shown in [40], Segre product is an example of a toric fiber product.

To that end, let  $A_X$  be the coordinate ring of  $X$ , and let  $I_{\boxtimes}$  be the defining ideal of the Segre product  $X \times X$ . Since the Lift operation preserves the squarefree binomial structure of Gröbner bases and the quadrics produced by Quad are differences of squarefree monomials, Theorem 5.2.1 implies that the ideal  $I_{\boxtimes}$  of the Segre product admits a squarefree initial ideal. Hence, Lemma 2.2.11 provides that the homogeneous coordinate rings  $A_X$  and  $A_X \boxtimes A_X$  are Cohen-Macaulay. By assumption, the dimension of  $X$  is at least one; thus the dimension of  $A_X$  is at least two. Now, we conclude by Lemma 5.2.3.  $\square$

In particular, the result holds for cut ideals. Note that the edge variety of a graph without edges is a point. Thus, it is harmless to restrict to graphs with at least one edge.

**Corollary 5.2.5.** *Let  $G$  be a graph with at least one edge whose cut ideal admits, for some monomial order, an initial ideal that is squarefree. Then the cut variety  $X_G$  is Hilbertian.*

### 5.3 Cut ideals of cycles

The starting point of this section is the realization of the cut ideals associated to cycles as certain phylogenetic ideals. This will enable us to use the main result from [11].

To establish this correspondence, we need some notation and recall the definition of certain ideals arising in phylogenetics. The claw tree  $K_{1,n}$  is the complete bipartite graph with  $n$  edges from one vertex (the root) to the other  $n$  vertices (the leaves). We denote by  $I_n$  the ideal of phylogenetic invariants for the general group-based model for the group  $\mathbb{Z}_2$  on the claw tree  $K_{1,n}$ , as in [11]. This ideal is the kernel of the following homomorphism between polynomial rings (see [19]):

$$\begin{aligned} \varphi_n : R := K[q_{g_1, \dots, g_n} : g_1, \dots, g_n \in \mathbb{Z}_2] &\rightarrow K[a_g^{(i)} : g \in \mathbb{Z}_2, i = 1, \dots, n+1] =: R' \\ q_{g_1, \dots, g_n} &\mapsto a_{g_1}^{(1)} a_{g_2}^{(2)} \dots a_{g_n}^{(n)} a_{g_1+g_2+\dots+g_n}^{(n+1)}. \end{aligned} \quad (*)$$

The coordinate  $q_{g_1, \dots, g_n}$  corresponds to observing the element  $g_1$  at the first leaf of the tree,  $g_2$  at the second, and so on, though here we are considering the phylogenetic ideals in Fourier coordinates instead of probability coordinates (cf. [?]).

We want to show that the cut ideal of an  $(n+1)$ -cycle is the same as the phylogenetic ideal  $I_n$  on the claw  $K_{1,n}$ , up to renaming the variables. Denote by  $C_{n+1}$  the  $(n+1)$ -cycle on the vertex set  $[n+1] := \{1, \dots, n+1\}$ . We are going to compare the above map  $\varphi_n$  with the map

$$\begin{aligned} \phi_{C_{n+1}} : S := K[q_{A|B} : A|B \text{ partition of } [n+1]] &\rightarrow K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } C_{n+1}] =: S', \\ q_{A|B} &\mapsto \prod_{\{i,j\} \in \text{Cut}(A|B)} s_{ij} \quad \prod_{\{i,j\} \in E(G) \setminus \text{Cut}(A|B)} t_{ij} \end{aligned}$$

In order to describe an isomorphism between the rings  $R$  and  $S$ , consider the map

$$\begin{aligned} \tilde{\gamma} : \{A|B : \text{partition of } [n+1]\} &\rightarrow (\mathbb{Z}_2)^n, \\ A|B &\mapsto (g_1, \dots, g_n), \end{aligned}$$

where

$$g_i = \begin{cases} 0 & \text{if } \{i, i+1\} \subset A \text{ or } \{i, i+1\} \subset B, \\ 1 & \text{otherwise} \end{cases}$$

One easily shows (for example, by induction on  $n$ ) that  $\tilde{\gamma}$  is bijective. Thus  $\tilde{\gamma}$  induces the ring isomorphism

$$\gamma : S \rightarrow R,$$

determined by

$$q_{A|B} \mapsto q_{g_1, \dots, g_n}, \text{ where } (g_1, \dots, g_n) := \tilde{\gamma}(A|B).$$

Now we are ready to state the announced comparison result.

**Lemma 5.3.1.** *Adopt the above notation. Then*

$$\gamma(\ker \varphi_{C_{n+1}}) = \ker \varphi_n,$$

that is, the phylogenetic ideal on the claw tree with  $n$  leaves and the cut ideal of an  $(n+1)$ -cycle agree up to renaming the variables using  $\tilde{\gamma}$ .

*Proof.* Consider the ring isomorphism

$$\delta : S' \rightarrow R',$$

which is induced by

$$\begin{aligned} t_{i, i+1} &\mapsto a_0^{(i)} \\ s_{i, i+1} &\mapsto a_1^{(i)}, \text{ if } 1 \leq i \leq n \end{aligned}$$

and

$$\begin{aligned} t_{n+1, 1} &\mapsto a_0^{(n+1)} \\ s_{n+1, 1} &\mapsto a_1^{(n+1)}. \end{aligned}$$



Our claim follows immediately, once we have shown that the following diagram is commutative:

$$\begin{array}{ccc} S & \xrightarrow{\varphi_{C_{n+1}}} & S' \\ \downarrow \gamma & & \downarrow \delta \\ R & \xrightarrow{\varphi_n} & R'. \end{array}$$

Comparing the definitions of the various maps, we see that it suffices to show that, for each partition  $A|B$ , the variable corresponding to the edge  $(n+1, 1)$  in the product  $\varphi(q_{A|B})$  is mapped by  $\delta$  onto  $a_{g_{n+1}}^{(n+1)}$ , where  $g_{n+1} = g_1 + \dots + g_n$  and  $(g_1, \dots, g_n) = \tilde{\gamma}(A|B)$ . To this end notice that  $g_{n+1} \in \mathbb{Z}_2$  is determined by  $g_1, \dots, g_n \in \mathbb{Z}_2$  such that  $g_1 + \dots + g_n + g_{n+1} = 0$  in  $\mathbb{Z}_2$ . Hence, to complete the argument, it is enough to show that the number of separating variables (i.e., the variables denoted by  $s$ ) that occur as a factor in  $\varphi(q_{A|B})$  is always even. But this is not difficult to see.

Indeed, if  $A = [n+1]$ , then there are no separating variables in  $\varphi(q_{A|B})$ . If  $A \neq [n+1]$ , then we think of  $A$  as the disjoint union of paths consisting of edges with both vertices in  $A$ . Using its endpoint(s), each such path gives rise to exactly two edges of  $C_{n+1}$  that correspond to separating variables in  $\varphi(q_{A|B})$ , and all separating variables occurring in  $\varphi(q_{A|B})$  arise in this manner. Hence, the number of separating variables that divide  $\varphi(q_{A|B})$  is even. This completes the proof.  $\square$

We illustrate the preceding proof by the simplest non-trivial example. Note that the phylogenetic ideal  $I_n$  is the zero ideal if  $n \in \{1, 2\}$ .

**Example 5.3.2.** Let  $n = 3$ . The phylogenetic ideal is  $I_3 = \ker \varphi_3$ , where the map  $\varphi_3$  is defined as follows:

$$\begin{array}{ll} \varphi_3 & : \quad K[q_{ijk} : i, j, k \in \{0, 1\}] \rightarrow K[a_0^{(1)}, a_0^{(2)}, a_0^{(3)}, a_0^{(4)}, a_1^{(1)}, a_1^{(2)}, a_1^{(3)}, a_1^{(4)}] \\ & q_{000} \mapsto a_0^{(1)} a_0^{(2)} a_0^{(3)} a_0^{(4)} \qquad q_{100} \mapsto a_1^{(1)} a_0^{(2)} a_0^{(3)} a_1^{(4)} \\ & q_{001} \mapsto a_0^{(1)} a_0^{(2)} a_1^{(3)} a_1^{(4)} \qquad q_{101} \mapsto a_1^{(1)} a_0^{(2)} a_1^{(3)} a_0^{(4)} \\ & q_{010} \mapsto a_0^{(1)} a_1^{(2)} a_0^{(3)} a_1^{(4)} \qquad q_{110} \mapsto a_1^{(1)} a_1^{(2)} a_0^{(3)} a_0^{(4)} \\ & q_{011} \mapsto a_0^{(1)} a_1^{(2)} a_1^{(3)} a_0^{(4)} \qquad q_{111} \mapsto a_1^{(1)} a_1^{(2)} a_1^{(3)} a_1^{(4)}. \end{array}$$

The cut ideal is  $I_{C_4} = \ker \phi_4$ , where

$$\begin{array}{ll} \phi_4 & : \quad K[q_{A|B} : A|B \text{ partition of } \{1, 2, 3, 4\}] \rightarrow K[t_{12}, t_{23}, t_{34}, t_{41}, s_{12}, s_{23}, s_{34}, s_{41}] \\ & q_{1|234} \mapsto t_{12} t_{23} t_{34} t_{41} \qquad q_{1|234} \mapsto s_{12} t_{23} t_{34} s_{41} \\ & q_{4|123} \mapsto t_{12} t_{23} s_{34} s_{41} \qquad q_{4|123} \mapsto s_{12} t_{23} s_{34} t_{41} \\ & q_{12|34} \mapsto t_{12} s_{23} t_{34} s_{41} \qquad q_{2|134} \mapsto s_{12} s_{23} t_{34} t_{41} \\ & q_{3|124} \mapsto t_{12} s_{23} s_{34} t_{41} \qquad q_{13|24} \mapsto s_{12} s_{23} s_{34} s_{41}. \end{array}$$

The above isomorphism  $\gamma$  identifies the variables  $q_{ijk}$  with  $q_{A|B}$  in the order listed above. It maps the cut ideal

$$I_{C_4} = (q_{1|234} q_{13|24} - q_{1|234} q_{3|124}, q_{1|234} q_{13|24} - q_{4|123} q_{2|134}, q_{1|234} q_{13|24} - q_{12|34} q_{13|23})$$

onto the phylogenetic ideal

$$I_3 = (q_{000}q_{111} - q_{100}q_{011}, q_{000}q_{111} - q_{010}q_{101}, q_{000}q_{111} - q_{001}q_{110}).$$

Recall that each toric ideal has a Gröbner basis consisting of binomials. We say that an ideal has a *squarefree Gröbner basis* if it has a Gröbner basis consisting of binomials, where *each* binomial is a difference of squarefree monomials. Note that this is a stronger condition than having a squarefree initial ideal.

Combining Lemma 5.3.1 and [11], Proposition 3, we obtain the following consequence.

**Proposition 5.3.3.** *For each integer  $n \geq 4$ , there is an order on the variables such that the cut ideal of the  $n$ -cycle has a quadratic squarefree Gröbner basis with respect to the resulting lexicographic order. In particular, the initial ideal of the cut ideal with respect to this order is squarefree.*

*Proof.* In case  $K = \mathbb{C}$ , Proposition 3 in [11] gives the analogous results for the phylogenetic ideal  $I_{k-1}$  on the claw tree with  $k - 1$  edges. The arguments of the proof are valid over an arbitrary field. Hence, the claim follows by Lemma 5.3.1.  $\square$

**Remark 5.3.4.** By [36], Corollary 2.4, the cut varieties defined by  $n$ -cycles are not smooth if  $n \geq 4$ .

Invoking Lemma 2.2.11, we obtain our first contribution to Conjecture 5.1.2.

**Corollary 5.3.5.** *The cut variety defined by any cycle is arithmetically Cohen-Macaulay.*

**Remark 5.3.6.** In general, cut ideals of cycles are not Gorenstein. However, the ideal  $I_{C_4}$  is Gorenstein because it is a complete intersection cut out by three quadrics.

We conclude this section by determining the number of minimal generators of the cut ideals of cycles. As preparation, we establish a recursion. Denote by  $A_n$  the homogeneous coordinate ring of the variety defined by the phylogenetic ideal  $I_n$ , that is,

$$A_n := K[a_{g_1}^{(1)} a_{g_2}^{(2)} \dots a_{g_n}^{(n)} a_{g_1+g_2+\dots+g_n}^{(n+1)} : g_i \in \mathbb{Z}_2, i = 1, \dots, n].$$

Assigning each variable degree one, as a  $K$ -algebra  $A_n$  is generated by  $2^n$  monomials of degree  $n + 1$ . We claim:

**Lemma 5.3.7.** *If  $n \geq 2$ , then*

$$\dim_K[A_n]_{2(n+1)} = \dim_K[A_{n-1}]_{2n} + 3^n - 2^{n-1}.$$

*Proof.* The following set of monomials is a  $K$ -basis of  $[A_n]_{2(n+1)}$ :

$$\mathcal{M} := \{a_{g_1}^{(1)} a_{h_1}^{(1)} \dots a_{g_n}^{(n)} a_{h_n}^{(n)} a_{g_1+\dots+g_n}^{(n+1)} a_{h_1+\dots+h_n}^{(n+1)} : g_j, h_j \in \mathbb{Z}_2\}.$$

We are going to compare this basis with the set of monomials

$$\mathcal{N} := \{a_{g_1}^{(1)} a_{h_1}^{(1)} \dots a_{g_n}^{(n)} a_{h_n}^{(n)} : g_j, h_j \in \mathbb{Z}_2\}.$$

Observing that, for the monomials in  $\mathcal{M}$ , the variables  $a_{g_1+\dots+g_n}^{(n+1)} a_{h_1+\dots+h_n}^{(n+1)}$  are determined by the remaining variables, one is tempted to guess that there is a bijection between  $\mathcal{M}$  and  $\mathcal{N}$ . However, this is not quite true. To illustrate this, consider the following example, where  $n = 3$ . Then, by interchanging the factors  $a_0^{(1)}$  and  $a_1^{(1)}$  in

$$m_1 := a_0^{(1)} a_0^{(2)} a_0^{(3)} a_1^{(1)} a_1^{(2)} a_0^{(3)} = a_1^{(1)} a_0^{(2)} a_0^{(3)} a_0^{(1)} a_1^{(2)} a_0^{(3)} =: m_2$$

this monomial in  $\mathcal{N}$  produces two different monomials in  $\mathcal{M}$ , namely

$$m_1 a_{0+0+0}^{(n+1)} a_{1+1+0}^{(n+1)} = m_1 a_0^{(n+1)} a_0^{(n+1)} \in [A_3]_8, \quad (\text{E})$$

$$m_2 a_{1+0+0}^{(n+1)} a_{0+1+0}^{(n+1)} = m_2 a_1^{(n+1)} a_1^{(n+1)} \in [A_3]_8. \quad (\text{O})$$

To keep track if a monomial in  $\mathcal{N}$  gives rise to one or two monomials in  $\mathcal{M}$  we use the following decomposition

$$\mathcal{N} = \mathcal{N}_1 \sqcup \mathcal{N}_2 \sqcup \mathcal{N}_3,$$

where

$$\mathcal{N}_1 := \{n \in \mathcal{N} : g_1 + \dots + g_n + h_1 + \dots + h_n = 1\}$$

$$\mathcal{N}_2 := \{n \in \mathcal{N} : n \text{ is a square}\}$$

$$\mathcal{N}_3 := \{n \in \mathcal{N} : g_1 + \dots + g_n + h_1 + \dots + h_n = 0, n \text{ is not a square}\}$$

The monomials in  $\mathcal{N}_1$  and  $\mathcal{N}_2$  give rise to just one monomial in  $\mathcal{M}$ , whereas the monomials in  $\mathcal{N}_3$  produce precisely two monomials in  $\mathcal{M}$  by interchanging the factors  $a_{g_i}^{(i)}$  and  $a_{h_i}^{(i)}$ , where  $g_i \neq h_i$ . This interchange alters the parity of  $g_1 + \dots + g_n = h_1 + \dots + h_n$ . It follows that

$$\begin{aligned} |\mathcal{M}| &= |\mathcal{N}_1| + |\mathcal{N}_2| + 2|\mathcal{N}_3| \\ &= |\mathcal{N}| + |\mathcal{N}'_3|, \end{aligned}$$

where

$$\mathcal{N}'_3 := \{n \in \mathcal{N} : g_1 + \dots + g_n = h_1 + \dots + h_n = 0, n \text{ is not a square}\}.$$

Each monomial in  $\mathcal{N}$  is the product of  $n$  quadratic monomials of the form  $a_{g_i}^{(i)} \cdot a_{h_i}^{(i)}$ , where  $g_i, h_i \in \mathbb{Z}_2$ . For fixed  $i$ , there are three such monomials, thus we get  $|\mathcal{N}| = 3^n$ , hence

$$|\mathcal{M}| = 3^n + |\mathcal{N}'_3|.$$

Notice that the condition  $g_1 + \dots + g_n = h_1 + \dots + h_n = 0$  is equivalent to  $g_1 + \dots + g_{n-1} = g_n$  and  $h_1 + \dots + h_{n-1} = h_n$ . It follows that the dimension of  $[A_{n-1}]_{2n}$  equals the sum of  $|\mathcal{N}'_3|$  and the number of squares  $n \in \mathcal{N}$  with  $g_1 + \dots + g_{n-1} = g_n$ . Since, there are  $2^{n-1}$  such squares, we obtain

$$\dim_K [A_n]_{2(n+1)} = |\mathcal{M}| = 3^n + \dim_K [A_{n-1}]_{2n} - 2^{n-1},$$

as claimed.  $\square$

Now we are ready to compute the number of minimal generators of a cut ideal associated to a cycle. Possibly, it is not too surprising that it has a nice combinatorial interpretation.

**Proposition 5.3.8.** *If  $n \geq 1$ , then the cut ideal of an  $n + 1$ -cycle is minimally generated by  $3 \cdot a(n + 1)$  quadratic binomials, where  $a(n) = \frac{1}{24}(4^n - 4(3^n) + 6(2^n) - 4)$  is the  $n^{\text{th}}$  Stirling number of the second kind.*

The numbers  $a(n)$  are the Stirling numbers  $S(n, 4)$  as defined, for example, in [12].

*Proof.* By Lemma 5.3.1, it is equivalent to compute the number of minimal generators of the phylogenetic ideal  $I_n$  corresponding to the claw tree  $K_{1,n}$ . Using the above notation,  $I_n$  is an ideal in the polynomial ring  $R$  with  $2^n$  variables. We first compute the Hilbert function of the quotient ring  $R/I_n$  in degree 2, that is,  $h_n(2) := \dim_K[R/I_n]_2$ . Since  $I_n = \ker \varphi_n$ , we get  $h_n(2) = \dim_K[A_n]_{2(n+1)}$ . Hence, Lemma 5.3.7 gives if  $n \geq 2$ :

$$h_n(2) = h_{n-1}(2) + 3^n - 2^{n-1}.$$

Using  $h_1(2) = 3$ , it follows that

$$\begin{aligned} h_n(2) &= h_1(2) + \sum_{i=2}^n 3^i - \sum_{i=1}^n 2^i \\ &= \frac{1}{2}[3^{n+1} - 1] - [2^n - 1] \\ &= \frac{3}{2}3^n - 2^n + \frac{1}{2}. \end{aligned}$$

Since, by Proposition 5.3.3, the ideal  $I_n$  is generated in degree two, its number  $\mu(I_n)$  of minimal generators is

$$\begin{aligned} \mu(I_n) &= \dim_K[R]_2 - h_n(2) \\ &= \binom{2^n + 1}{2} - \frac{3}{2}3^n + 2^n - \frac{1}{2} \\ &= \frac{1}{2}4^n - \frac{3}{2}3^n + \frac{3}{2}2^n - \frac{1}{2}. \end{aligned}$$

It is easily checked that the last number equals  $3a(n + 1)$ . The proof is complete.  $\square$

## 5.4 Cut ideals of trees

The goal of this section is to show that algebraic properties of cut ideals associated to trees only depend on the number of edges and not on the specific structure of the tree. We use this to establish that the resulting cut ideals are Gorenstein and to compute

their  $h$ -vector. It turns out that its entries admit combinatorial interpretations. We begin with a more general result that applies to any graph with a leaf. Roughly speaking, it says that moving the leaf essentially does not change the cut ideal. Let  $G$  be a tree with at least one edge, say  $\{p_1, p_2\}$ . Let us add a new vertex  $r$  and an edge to  $G$  in two ways: Let  $G_1$  and  $G_2$  be the graph obtained from  $G$  by adding a new edge  $\{p_1, r\}$  and  $\{p_2, r\}$ , respectively. In order to compare the corresponding cut ideals  $I_{G_1}$  and  $I_{G_2}$  we need some notation.

We want to define a map  $\tilde{\gamma}$  between the set of partitions of the vertex set of  $G_1$

$$\tilde{\gamma} : \{A|B \text{ partition of } V(G_1)\} \rightarrow \{A|B \text{ partition of } V(G_1)\}.$$

To this end we distinguish three cases. Recall that we always consider unordered partitions.

**Case I** If  $\{p_1, p_2\} \subset A$ , then we set  $\tilde{\gamma}(A|B) := A|B$ .

**Case II** If  $\{p_1, r\} \subset A$  and  $\{p_2\} \subset B$ , then we define  $\tilde{\gamma}(A|B) := C|D$ , where  $C := A \setminus \{r\}$  and  $D := B \cup \{r\}$ .

**Case III** If  $\{r, p_2\} \subset A$  and  $\{p_1\} \subset B$ , then we define  $\tilde{\gamma}(A|B) := C|D$ , where  $C := A \setminus \{r\}$  and  $D := B \cup \{r\}$ .

Clearly, the map  $\tilde{\gamma}$  is bijective. It induces the ring isomorphism

$$\gamma : S = K[q_{A|B} : A|B \text{ is partition of } V(G_1)] \rightarrow S,$$

which is induced by

$$\gamma(q_{A|B}) := q_{\tilde{\gamma}(A|B)}.$$

It allows us to compare the two cut ideals. Since  $G_1$  and  $G_2$  are 0-sums of  $G$  and an edge, their cut varieties are isomorphic. However, more is true, and this allows us to compare Gröbner bases of cut ideals of trees.

**Lemma 5.4.1.** *Using the above notation,*

$$\gamma(\ker \varphi_{G_1}) = \ker \varphi_{G_2},$$

*that is, the cut ideals  $I_{G_1}$  and  $I_{G_2}$  agree up to renaming the variables using  $\tilde{\gamma}$ .*

*Proof.* In order to relate the maps  $\varphi_{G_1}$  and  $\varphi_{G_2}$ , consider the algebra homomorphism

$$\delta : S' := K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } G_1] \rightarrow S'' := K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } G_2]$$

induced by

$$\delta(s_{ij}) := \begin{cases} s_{p_2, r} & \text{if } \{i, j\} = \{p_1, r\} \\ s_{ij} & \text{otherwise;} \end{cases}$$

and

$$\delta(t_{ij}) := \begin{cases} t_{p_2, r} & \text{if } \{i, j\} = \{p_1, r\} \\ t_{ij} & \text{otherwise.} \end{cases}$$

Since  $\{p_2, r\}$  is an edge of  $G_2$ , but not of  $G_1$ , the map  $\delta$  is well-defined. It is an algebra isomorphism. Hence our claim follows, once we have shown that the following diagram is commutative:

$$\begin{array}{ccc} S & \xrightarrow{\varphi_{G_1}} & S' \\ \downarrow \gamma & & \downarrow \delta \\ S & \xrightarrow{\varphi_{G_2}} & S'' \end{array}$$

However, this is easily checked for each of the variables  $q_{A|B}$  by distinguishing the Cases I-III considered above.  $\square$

The above result allows us to identify the cut ideals of trees.

**Theorem 5.4.2.** *Let  $T$  be a tree with  $n \geq 1$  edges, and let  $X_T \subset \mathbb{P}^{2^n-1}$  be the toric variety defined by the cut ideal  $I_T$ . Then  $X_T$  is arithmetically Cohen-Macaulay of dimension  $n$  and degree  $n!$ . More precisely,  $X_T$  is isomorphic to the Segre embedding of  $(\mathbb{P}^1)^n$  into  $\mathbb{P}^{2^n-1}$  and its Hilbert function is*

$$h_{S_T/I_T}(i) = (i+1)^n \quad (i \geq 0).$$

*Proof.* Applying Lemma 5.4.1 repeatedly, we see that the cut ideal of  $T$  is isomorphic to the cut ideal of a path  $P_n$  with  $n$  edges. Its cut ideal  $I_{P_n}$  is an ideal in the polynomial ring, say  $S_n$ , with  $2^n$  variables. As mentioned in [36],  $P_n$  can be constructed from  $P_1$  by repeated use of the 0-sum construction. In fact,  $P_n$  is the zero sum of  $P_{n-1}$  and  $P_1$ . Since 0-sums of graphs correspond to Segre products of the coordinate rings, it follows that  $S_n/I_{P_n} = S_{n-1}/I_{P_{n-1}} \boxtimes S_1/I_{P_1}$ . But  $I_{P_1} = 0$ , so  $S_1/I_{P_1} = S_1 = K[q_{1|2}, q_{1|2}]$ , and thus

$$S_n/I_{P_n} = \underbrace{S_1 \boxtimes \cdots \boxtimes S_1}_{n \text{ times}}.$$

The Segre product of projective spaces is arithmetically Cohen-Macaulay. Thus, we see that  $X_T$  is arithmetically Cohen-Macaulay and isomorphic to the claimed Segre embedding.

The Hilbert function of a Segre product is the product of the Hilbert functions of the factors:

$$h_{A \boxtimes B}(i) = h_A(i)h_B(i).$$

Thus, the Hilbert function of the coordinate ring of  $X_T$  is, for all integers  $i \geq 0$ ,

$$h_{S_n/I_{P_n}}(i) = (i+1)^n,$$

as claimed.  $\square$

Again, we see that the number of minimal generators of a cut ideal grows rapidly when the number of edges increases.

**Corollary 5.4.3.** *If  $T$  is a tree with  $n$  edges, then its cut ideal is minimally generated by  $2 \cdot 4^{n-1} + 2^{n-1} - 3^n$  quadrics.*

*Proof.* As noted above, the cut ideal  $I_T$  lies in a polynomial ring  $S_n$  with  $2^n$  variables. Using that  $h_{S_n/I_T}(2) = 3^n$  by the above theorem, the claim follows.  $\square$

The next result provides in particular that the cut ideal of a tree has a minimal generating set that is even a Gröbner basis. Note that the cut ideal of a tree with one edge is trivial.

**Proposition 5.4.4.** *If  $T$  is a tree with a least two edges, then there is a monomial order such that its cut ideal has a quadratic squarefree Gröbner basis. In particular, the corresponding initial ideal is squarefree.*

*Proof.* This follows by Theorem 5.2.1 as the Lift and Quad operations preserve the squarefree structure and degree of the binomials.  $\square$

Our next goal is to make the Hilbert series of the cut variety of a tree explicit. We will see that it admits a combinatorial interpretation. For a positive integer  $n$ , denote by  $\mathcal{S}_n$  the symmetric group on  $n$  letters. The  $n^{\text{th}}$  Eulerian polynomial  $A_n$  is defined as

$$A_n(t) := \sum_{\sigma \in \mathcal{S}_n} t^{1+d(\sigma)},$$

where  $d(\sigma)$  is the number of descents of the permutation  $\sigma$  (see, e.g., [33], page 22). Writing

$$A_n(t) = A_{n,1}t + \cdots + A_{n,n}t^n,$$

the coefficients  $A_{n,k}$  are called *Eulerian numbers*. Like binomial coefficients, they satisfy a recurrence relation:

$$A_{n,i+1} = (n-i)A_{n-1,i} + (i+1)A_{n-1,i+1}.$$

For trees, the above concept is related to the  $h$ -vector:

**Proposition 5.4.5.** *Let  $T$  be a tree with  $n \geq 1$  edges. Then the Hilbert series of its cut variety  $X_T$  is*

$$h(X_T) = \frac{A_{n,1} + A_{n,2}t + \cdots + A_{n,n}t^{n-1}}{(1-t)^{n+1}}.$$

Moreover, the Castelnuovo-Mumford regularity is  $\text{reg } X = n$ .

*Proof.* By Theorem 5.4.2, we know that the Hilbert series of  $X$  is

$$H_X(t) = \sum_{i \geq 0} (i+1)^n t^i.$$

It is known (see, for example, [33], page 209, or [12]) that the Eulerian polynomials satisfy

$$\sum_{i \geq 0} i^n t^i = \frac{A_n(t)}{(1-t)^{n+1}}.$$

Dividing by  $t$  provides the desired formula for the Hilbert series of  $X$ .

Finally, since  $X$  is arithmetically Cohen-Macaulay, the regularity of its homogeneous coordinate ring is the degree of the numerator polynomial in the Hilbert series. Hence  $A_{n,n} = 1$  provides  $\text{reg } X = n$ .  $\square$

The *Eulerian number*  $A_{n,k}$  equals the number of permutations in  $\mathcal{S}_n$  with  $k-1$  excedances (see [33], Proposition 1.3.12). It follows that

$$A_{n,k} = A_{n,n+1-k}. \quad (5.1)$$

This allows us to strengthen the Cohen-Macaulay property established in Theorem 5.4.2.

**Corollary 5.4.6.** *The cut variety of any tree or, equivalently,  $\mathbb{P}^1 \times \cdots \times \mathbb{P}^1$  is arithmetically Gorenstein.*

*Proof.* A theorem of Stanley [32] (see also [7], Corollary 4.4.6) says that a standard graded Cohen-Macaulay domain is Gorenstein if and only if its  $h$ -vector is symmetric. Hence, the assertion follows by Proposition 5.4.5 and Equation (5.1).  $\square$

## 5.5 Disjoint unions

We want to show that the cut ideal of a disjoint union of two graphs can be studied by means of their zero-sum. We need a general fact:

**Lemma 5.5.1.** *Let  $R = K[x_1, \dots, x_n]$  and  $S := K[x_1, \dots, x_n, y_1, \dots, y_n]$  be polynomial rings in  $n$  and  $2n$  variables, respectively. Let  $\psi : R \rightarrow T$  be any  $K$ -algebra homomorphism and consider the homomorphism  $\varphi : S \rightarrow T$  that is defined by  $\varphi(y_i) = \varphi(x_i) := \psi(x_i)$ ,  $i = 1, \dots, n$ . Set  $I := \ker \varphi$  and  $J := \ker \psi$ . Then*

$$I = J \cdot S + (x_1 - y_1, \dots, x_n - y_n)$$

and  $S/I \cong R/J$ .

Moreover, if, for some monomial order on  $R$ ,  $\mathbf{F}$  is a Gröbner basis of  $J$ , then  $\mathbf{F} \cup \{x_1 - y_1, \dots, x_n - y_n\}$  is a Gröbner basis of  $I$  with respect to some monomial order on  $S$ .

*Proof.* This is probably well-known to specialists. For the convenience of the reader we provide a short proof. The  $K$ -algebra homomorphism  $\gamma : S \rightarrow R$  that maps



$x_i$  and  $y_i$  onto  $x_i$  induces the following commutative diagram with exact rows and column

$$\begin{array}{ccccccc}
& & & & 0 & & \\
& & & & \downarrow & & \\
& & & & L & & \\
& & & & \downarrow & & \\
0 & \longrightarrow & I & \longrightarrow & S & \xrightarrow{\varphi} & T \\
& & \downarrow & & \downarrow \gamma & & \downarrow = \\
0 & \longrightarrow & J & \longrightarrow & R & \xrightarrow{\psi} & T, \\
& & & & \downarrow & & \\
& & & & 0 & & 
\end{array}$$

where  $L$  is the ideal  $L := (x_1 - y_1, \dots, x_n - y_n)$ . Thus, we get an exact sequence

$$0 \rightarrow L \rightarrow I \rightarrow J \rightarrow 0.$$

Using also the natural embedding of  $R$  as a subring of  $S$ , we conclude that  $I = J \cdot S + L$ , as desired.

The claim about the Gröbner bases follows by using an elimination order on  $S$  that extends the term order on  $R$  used for computing the Gröbner basis  $\mathbf{F}$  with the property that each variable  $y_1 > y_2 > \dots > y_n$  is greater than any monomial in  $R$ .  $\square$

Let  $G_1$  and  $G_2$  be (non-empty) graphs on  $v_1$  and  $v_2$  vertices. Consider the zero-sum  $G_0 := G_1 \# G_2$  obtained by joining the two graphs at any vertex. Its cut ideal lies in a polynomial ring  $R$  with  $2^{v_1+v_2-1}$  variables. The disjoint union of the two graphs  $G_{\sqcup} := G_1 \sqcup G_2$  defines a cut ideal in a polynomial ring  $S$  in  $2^{v_1+v_2}$  variables. Using this notation, the main result of this section is:

**Proposition 5.5.2.** *There is an injective, graded  $K$ -algebra homomorphism  $\alpha : R \rightarrow S$  mapping the variables of  $R$  onto variables of  $S$  such that*

$$I_{G_1 \sqcup G_2} = \alpha(I_{G_0}) + L,$$

where  $L \subset S$  is an ideal that is minimally generated by  $2^{v_1+v_2-2}$  linear forms. Furthermore, the cut variety  $X_{G_1 \sqcup G_2} \subset \mathbb{P}^{2^{v_1+v_2}-1}$  is isomorphic to the Segre embedding of  $X_{G_1} \times X_{G_2}$  into  $\mathbb{P}^{2^{v_1+v_2}-1}$ .

*Proof.* To simplify notation, set  $G_{\sqcup} := G_1 \sqcup G_2$ . Moreover, denote the polynomial rings that are used to define cut ideals of  $G_{\sqcup}$  and the zero sum  $G_0$  by  $S, S', R, R'$ , that is,  $I_{G_{\sqcup}}$  is the kernel of  $\varphi_{G_{\sqcup}} : S \rightarrow S'$  and  $I_{G_0}$  is the kernel of  $\varphi_{G_0} : R \rightarrow R'$ . Let  $x \in V(G_1)$  and  $y \in V(G_2)$  be the vertices of  $G_1$  and  $G_2$  that are identified in

the 0-sum  $G_0$ . It will be convenient to denote the resulting vertex in  $G_0$  by  $z$ . There is a natural bijection  $\tilde{\beta} : E(G_0) \rightarrow E(G_\sqcup)$ , defined by

$$\{i, j\} \mapsto \tilde{\beta}(\{i, j\}) := \begin{cases} \{i, j\} & \text{if } z \notin \{i, j\}, \\ \{i, x\} & \text{if } j = z, i \in G_1, \\ \{i, y\} & \text{if } j = z, i \in G_2. \end{cases}$$

It induces an isomorphism  $\beta : R' \rightarrow R$ .

Now consider any unordered partition  $A|B$  of the vertex set of  $G_0$ . We may assume that  $z \in A$ . Then we define a partition  $A'|B$  of the vertex set of  $G_\sqcup$  by setting  $A' := (A \setminus \{z\}) \cup \{x, y\}$ . This induces an injective  $K$ -algebra homomorphism  $\alpha : R \rightarrow S$  that maps the variable  $q_{A|B} \in R$  onto the corresponding variable  $q_{A'|B} \in S$ .

Observing that  $\tilde{\beta}$  maps  $\text{Cut}(A|B)$  onto  $\text{Cut}(A'|B)$ , we get a commutative diagram

$$\begin{array}{ccc} R & \xrightarrow{\varphi_{G_0}} & R' \\ \downarrow \alpha & & \downarrow \beta \\ S & \xrightarrow{\varphi_{G_\sqcup}} & S'. \end{array}$$

Since  $\alpha$  is injective, it follows immediately that  $J := \alpha(I_{G_0}) \subset I_{G_\sqcup}$ .

We now consider the set  $\mathcal{P}$  of partitions of the vertex set of  $G_\sqcup$ . We decompose it as

$$\mathcal{P} = \mathcal{P}_1 \sqcup \mathcal{P}_2,$$

where

$$\mathcal{P}_1 := \{A|B \in \mathcal{P} : x, y \in A\}$$

and

$$\mathcal{P}_2 := \{A|B \in \mathcal{P} : x \in A, y \in B\}$$

Given a partition  $A|B \in \mathcal{P}_1$ , define sets  $C, D$ :

$$C := (A \cap V(G_1)) \cup (B \cap V(G_2))$$

$$D := (B \cap V(G_1)) \cup (A \cap V(G_2)).$$

Then  $C|D$  is a partition in  $\mathcal{P}_2$ , thus we get a map  $\varepsilon : \mathcal{P}_1 \rightarrow \mathcal{P}_2$ . Note that this map is bijective, thus  $|\mathcal{P}_1| = \frac{1}{2}|\mathcal{P}| = 2^{v_1+v_2-1}$ . Moreover, the cut sets of  $A|B \in \mathcal{P}_1$  and  $C|D = \varepsilon(A|B)$  are the same. Using also that  $\alpha$  maps the variables in  $R$  onto variables in  $S$  indexed by partitions in  $\mathcal{P}_1$ , Lemma 5.5.1 provides

$$I_{G_\sqcup} = J + (q_{A|B} - q_{\varepsilon(A|B)}) : A|B \in \mathcal{P}_1 \tag{5.2}$$

and an isomorphisms between the homogeneous coordinate rings of the cut varieties defined by  $G_\sqcup$  and  $G_0$ . Since taking 0-sums corresponds to forming Segre products, it follows that  $X_{G_\sqcup} \cong X_{G_1} \times X_{G_2}$ , and the proof is complete.  $\square$

The above proof also implies:

**Corollary 5.5.3.** *If the cut ideals of  $G_1$  and  $G_2$  admit a squarefree Gröbner basis, then so does the cut ideal of their disjoint union.*

*Proof.* The assumption implies that the cut ideal of the zero sum of  $G_1$  and  $G_2$  admits a squarefree Gröbner basis. Hence, using the second assertion of Lemma 5.5.1, Equation (5.2) provides the claim.  $\square$

Now we address the transfer of the Cohen-Macaulay property under forming disjoint unions.

**Corollary 5.5.4.** *Let  $G_1$  and  $G_2$  be two graphs such that their cut varieties are arithmetically Cohen-Macaulay. Then the cut variety associated to the disjoint union of  $G_1$  and  $G_2$  is arithmetically Cohen-Macaulay if and only if the two varieties defined by  $G_1$  and  $G_2$  are Hilbertian.*

*Proof.* Denote by  $T, T_1$ , and  $T_2$  the homogeneous coordinate rings of the cut varieties associated to  $G_1 \sqcup G_2, G_1$ , and  $G_2$ , respectively. Proposition 5.5.1 provides that  $T$  is isomorphic to the Segre product  $T_1 \boxtimes T_2$ . If, say,  $G_1$  does not have any edge, then  $T_1$  is isomorphic to a polynomial ring in one variable. Thus it is Hilbertian and  $T$  is isomorphic to  $T_2$ .

If both graphs  $G_1$  and  $G_2$  have at least one edge, the Krull dimension of  $T_1$  and  $T_2$  is at least two. Then the claim is a consequence of Lemma 5.2.3.  $\square$

Recall that a *forest* is a disjoint union of trees. We get the following generalization of Corollary 5.4.6:

**Corollary 5.5.5.** *The cut variety defined by any forest is arithmetically Gorenstein.*

*Proof.* This follows immediately by combining Corollary 5.4.6 and Proposition 5.5.2.  $\square$

## 5.6 Cut ideals of series-parallel graphs

Recall that simple series-parallel graphs are precisely the graphs free of  $K_4$  minors. Trees and cycles are examples of such graphs. With Conjecture 5.1.1 in mind, we will first obtain quadratic squarefree Gröbner bases for *ring graphs*, which form a large subclass of series-parallel graphs and can be obtained from trees and cycles. Then, we will complete the proof of the quadratic generation conjecture (5.1.1) by studying the remaining series-parallel graphs.

Let us begin with ring graphs. To define them, we need some vocabulary. A vertex  $v$  of a graph  $G$  is called a *cutvertex* if the number of connected components of  $G \setminus \{v\}$  is larger than that of  $G$ . Similarly, an edge  $e$  is called a *bridge* if the number of connected components of  $G \setminus \{e\}$  is larger than that of  $G$ . A *block* of  $G$  is a maximal connected subgraph of  $G$  without cut vertices. A graph is *2-connected* if it has at least two vertices and has no cut vertices. It follows that each block of  $G$  is either an isolated vertex, a bridge, or a maximal 2-connected subgraph.

The following definition can be found in [41] or [16]:

**Definition 5.6.1.** A *ring graph* is a graph  $G$  with the property that each block of  $G$  which is not a bridge or a vertex can be constructed from a cycle by successively adding cycles of length at least 3 using the edge-sum (1-sum) construction.

Examples of ring graphs include trees and cycles. More precisely, ring graphs are those graphs that can be obtained from trees and cycles by performing clique sums over vertices or edges. Thus, combining our results from the previous sections, we obtain the following:

**Theorem 5.6.2.** *If  $G$  is a ring graph, then the cut variety  $X_G$  is generated by quadrics. In addition, there exists a term order for which its defining ideal  $I_G$  has a squarefree quadratic Gröbner basis.*

*Therefore, such varieties  $X_G$  are Hilbertian and arithmetically Cohen-Macaulay, but not Gorenstein in general.*

*Proof.* The result follows by combining Proposition 5.3.3, Theorem 5.4.2, and Theorem 5.2.1 repeatedly.  $\square$

Recall that if an ideal  $I$  admits a quadratic Gröbner basis, then the coordinate ring  $S/I$  is Koszul. We have just found another infinite family of toric varieties whose coordinate rings  $S/I$  are G-quadratic.

**Corollary 5.6.3.** *The coordinate ring of the cut variety associated to each ring graph is Koszul.*

**Remark 5.6.4.** Theorem 1.3. of [36] characterizes those graphs whose cut ideals have squarefree reverse-lexicographic initial ideals. Arbitrary ring graphs *do not* fall into that category, however our result shows that they *do* have squarefree initial ideals with respect to another term order.

From [41] we know that ring graphs form a large subclass of series-parallel graphs. More precisely, a graph  $G$  is a ring graph if and only if it is free of  $K_4$ -minors and it satisfies the *primitive cycle property*: any two cycles of  $G$  share at most one edge. Essentially, ring graphs are those simple series-parallel graphs for which we restrict certain series extensions: we do not allow subdivisions of edges along which edge-sums are performed.

Let us return to the primitive cycle property. Suppose there are two cycles  $C_1$  and  $C_2$  in a simple series-parallel graph  $G$  that share two *nonadjacent* edges, say  $e_1$  and  $e_2$ . Let  $P$  be the planar presentation of the two cycles in  $G$ . The two common edges of  $C_1$  and  $C_2$  divide the remaining edges into two groups: those whose endvertices are on the outer face of  $P$  are separated from the remaining edges by  $e_1$  and  $e_2$ . Clearly, the edges that do not have endvertices on the outer face form another cycle, say  $C_3$ . Thus, any two such cycles  $C_1$  and  $C_2$  which share two nonadjacent edges can be interpreted as three cycles,  $C_1$ ,  $C_3$  and  $C_2$ , which share *adjacent* edges. This argument can be generalized to cycles that share any number of nonadjacent edges.

Therefore, to complete the study of cut ideals of graphs free of  $K_4$ -minors, it suffices to study the cut ideals of graphs which are obtained from a cycle by successively

attaching cycles of arbitrary length. We will call any such graph a *path-sum* of a cycle and another graph; that is,  $G$  is a path-sum if it consists of a smaller graph and a cycle which share a common path. The cycles in  $G$ , as well as the paths they share, can be of arbitrary and unequal lengths. We will study such graphs by reducing to a simpler case. To that end, we establish an isomorphism between ideals which are obtained by path-sums with cycles of fixed lengths. Clearly, we may restrict our study to path-sums along paths of length at least two.

We begin with a general construction which mimics that of Section 5.4. Consider a graph  $G$  which contains a  $k$ -path, so that  $G$  contains edges  $\{p_1, p_2\}, \{p_2, p_3\}, \dots, \{p_{k-1}, p_k\}$ , for  $k \geq 2$ . For an arbitrary integer  $n$ , we will create two new graphs by taking a path-sum with an  $(n+k-1)$ -cycle containing new vertices  $r_1, \dots, r_n \notin V(G)$  along the two  $(k-1)$ -paths in  $G$ . More precisely, let  $G_1$  be the path-sum of  $G$  and the cycle

$$p_1, r_1, \dots, r_n, p_{k-1}, p_{k-2}, \dots, p_1$$

along the path  $p_1, \dots, p_{k-1}$ ; and let  $G_2$  be the path-sum of  $G$  and the cycle

$$p_2, r_1, \dots, r_n, p_k, p_{k-1}, \dots, p_2$$

along the path  $p_2, \dots, p_k$ .

We want to define a map  $\tilde{\gamma}$  between the sets of partitions of the vertex sets of  $G_1$  and  $G_2$ :

$$\tilde{\gamma} : \{A|B \text{ partition of } V(G_1)\} \rightarrow \{A|B \text{ partition of } V(G_2)\}.$$

Note that the vertex sets of the two graphs are equal, however we would like to think of the map  $\tilde{\gamma}$  this way for reasons that will become clear shortly. To this end, we need to distinguish two cases:

**Case I** Suppose that  $p_1$  and  $p_{k-1}$  are both in  $A$  or both in  $B$ , and the same holds for  $p_2$  and  $p_k$ , or if  $p_1$  and  $p_{k-1}$  are not both in  $A$  and not both in  $B$ , and the same holds for  $p_2$  and  $p_k$ . Then if  $p_1$  and  $p_2$  are both in  $A$  or both in  $B$ , we set

$$\tilde{\gamma}(A|B) := A|B.$$

If on the other hand  $p_1 \in A$  and  $p_2 \in B$  or vice versa, we define  $R_A := A \cap \{r_1, \dots, r_n\}$  and  $R_B := B \cap \{r_1, \dots, r_n\}$ . Note that  $R_A$  and  $R_B$  simply record the locations of the new vertices  $r_1, \dots, r_n$ . Then, we set

$$\tilde{\gamma}(A|B) := C|D,$$

where

$$C := A \setminus R_A \cup R_B$$

and

$$D := B \setminus R_B \cup R_A.$$

**Case II** Suppose that  $p_1$  and  $p_{k-1}$  are both in  $A$  or both in  $B$  while  $p_2$  and  $p_k$  are not, or vice versa:  $p_1$  and  $p_{k-1}$  are not both in  $A$  and not both in  $B$ , while  $p_s$  and  $p_k$  are both in  $A$  or in  $B$ . Define  $V_A := A \cap \{p_2, \dots, p_{k-1}, r_1, \dots, r_n\}$  and  $V_B := B \cap \{p_2, \dots, p_{k-1}, r_1, \dots, r_n\}$ . Then we set

$$\tilde{\gamma}(A|B) := C|D,$$

where

$$C := A \setminus V_A \cup V_B$$

and

$$D := B \setminus V_B \cup V_A.$$

Clearly, the map  $\tilde{\gamma}$  is bijective and induces an isomorphism  $\gamma$  between the polynomial rings corresponding to the two cut varieties, which is induced by

$$\gamma : K[q_{A|B} : A|B \text{ is partition of } V(G_1)] \rightarrow K[q_{A|B} : A|B \text{ is partition of } V(G_2)],$$

$$\gamma(q_{A|B}) := q_{\tilde{\gamma}(A|B)}.$$

**Lemma 5.6.5.** *Using the above notation,*

$$\gamma(\ker \varphi_{G_1}) = \ker \varphi_{G_2},$$

that is, the cut ideals  $I_{G_1}$  and  $I_{G_2}$  agree up to renaming variables using  $\tilde{\gamma}$ .

*Proof.* The proof is identical to that of Lemma 5.4.1 after we redefine the map  $\delta$ :

$$\delta : S' := K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } G_1] \rightarrow S'' := K[s_{ij}, t_{ij} : \{i, j\} \text{ edge of } G_2].$$

The algebra homomorphism  $\delta$  is induced by

$$\delta(s_{ij}) := \begin{cases} s_{p_{k-m}, p_{k-m+1}} & \text{if } \{i, j\} = \{m, m+1\} \text{ for } 1 \leq m \leq k-1, \\ s_{p_2, r_1} & \text{if } \{i, j\} = \{p_1, r_1\}, \\ s_{p_k, r_n} & \text{if } \{i, j\} = \{p_{k-1}, r_n\}, \\ s_{ij} & \text{otherwise,} \end{cases}$$

and

$$\delta(t_{ij}) := \begin{cases} t_{p_{k-m}, p_{k-m+1}} & \text{if } \{i, j\} = \{m, m+1\} \text{ for } 1 \leq m \leq k-1, \\ t_{p_2, r_1} & \text{if } \{i, j\} = \{p_1, r_1\}, \\ t_{p_k, r_n} & \text{if } \{i, j\} = \{p_{k-1}, r_n\}, \\ t_{ij} & \text{otherwise.} \end{cases}$$

□

We are now ready to prove the quadratic generation conjecture:

**Theorem 5.6.6.** *The cut ideal of  $G$  is generated by quadrics if and only if  $G$  is free of  $K_4$ -minors.*

*Proof.* The necessary condition is stated in [36], where it is shown that the cut ideal of  $K_4$  has a minimal generator of degree four.

It remains to prove sufficiency. Let  $G$  be a graph free of  $K_4$ -minors. Then each block of  $G$  which is not a bridge or a vertex can be constructed from a cycle by successively adding path-sums with cycles. Our results on quadratic generation of cut ideals of trees (5.3.3) and cycles (5.4.2), together with the clique-sum construction of Sturmfels and Sullivant (5.2.1), reduce the study of  $K_4$ -free graphs to path-sums of cycles.

The simplest example of a path-sum of cycles is a *subdivision of a book*: it is simply constructed as a path-sum of cycles of arbitrary lengths with the property that all cycles share *the same* path. Using our constructions defined for Lemma 5.6.5, each path-sum  $P$  of cycles can be deformed to another path-sum  $P'$  of cycles with the additional property that each path in  $P'$  shared by two cycles has at least one edge not shared with any other cycles. Lemma 5.6.5 provides an isomorphism between the two cut ideals  $I_P$  and  $I_{P'}$ .

Further, note that we may subdivide those edges not shared by more than two cycles until all shared paths are of *the same length*. Denote the graph obtained in this way by  $P'_c$ . Recall from Corollary 3.3 in [36] that contracting edges does not increase degrees of minimal generators of cut ideals. Hence, if the cut ideal of  $P'_c$  is generated by quadrics, then so is the cut ideal of  $P'$  and, consequently, the cut ideal of  $P$  as well.

Further repeated applications of Lemma 5.6.5 provide that the cut ideal of every such graph  $P'_c$  is isomorphic to the cut ideal of a subdivision of a book. Now we use the main result of Brennan and Chen in [6], which states that cut ideals of subdivisions of books are generated in degree two.

Therefore, Conjecture 5.1.1 is true. □

This concludes our study of cut ideals. However, as many open questions remain, further investigations will appear in the forthcoming paper [28].

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