Algebraic and Combinatorial Aspects of Group-Based Models

Kaie Kubjas

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Eidesstattliche Erklärung

Gemäß §7 (4) der Promotionsordnung des Fachbereichs Mathematik und Informatik der Freien Universität Berlin versichere ich hiermit, dass ich alle Hilfsmittel und Hilfen angegeben und auf dieser Grundlage die Arbeit selbständig verfasst habe. Des Weiteren versichere ich, dass ich diese Arbeit nicht schon einmal zu einem früheren Promotionsverfahren eingereicht habe.

Berlin, den

Kaie Kubjas

Preface

The aim of this thesis is to study discrete structures associated with group-based models. Group-based models are statistical models on phylogenetic trees that can be parametrized by polynomial maps. The algebraic varieties given by these polynomial maps are toric. By the well-known correspondence between toric varieties and polyhedral fans, we can associate discrete structures, such as lattice polytopes and affine semigroups, with group-based models.

We follow three main lines in this dissertation. In Chapters 2 and 3, we study the Hilbert polynomials of group-based models. This is motivated by a result of Buczyńska and Wiśniewski stating that the Hilbert polynomial of the Jukes-Cantor binary model on a trivalent tree does not depend on the shape of the tree [BW07]. In Chapter 2, we give a simple combinatorial proof to this statement, and in Chapter 3, we show that the analogous statement does not hold for the Kimura 3-parameter model.

In Chapters 4 and 5, we study the phylogenetic semigroups on graphs that generalize the Jukes-Cantor binary model on trees [Buc12, BBKM11]. In Chapter 4, we study the maximal degrees of the minimal generators of these semigroups. In Chapter 5, we investigate the minimal generators of the phylogenetic semigroups on graphs with a few holes, extending the work of Buczyńska [Buc12].

Finally, in Chapter 6, we establish a connection between Berenstein-Zelevinsky triangles from representation theory and group-based models. This is motivated by the recent work of Sturmfels, Xu, and Manon related to conformal block algebras [SX10, Man09, Man12a].

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I would like to dedicate this dissertation to my parents and my brother for their all-encompassing support.

Contents

Introduction

Algebraic statistics uses algebro-geometric and combinatorial methods to study problems in statistics. As a side effect, algebraic statistics leads to advances in algebraic geometry and combinatorics. One of the first articles in algebraic statistics was [DS98] by Diaconis and Sturmfels in 1998. Since then the development of the field has been rapid and several books have been written [PRW01, PS05, DSS09, Wat09].

Phylogenetic algebraic geometry is part of algebraic statistics that explores phylogenetic statistical models on trees. Phylogenetics is the study of evolution of species based on genetic information, see [Fel04, SS05a]. Phylogenetic models on trees can be parametrized by polynomial maps. Hence, there are algebraic varieties associated with them, which are main objects of study in phylogenetic algebraic geometry.

Group-based models are special phylogenetic models that are invariant under the action of an abelian group. They are especially interesting to combinatorialists, because algebraic varieties associated with them are toric varieties [ES93, SSE93]. There is a well-known correspondence between toric varieties and discrete structures, such as affine semigroups and lattice polytopes. The central theme of this dissertation is the study of these discrete structures associated with group-based models.

The starting points of this dissertation are two results by Buczyńska and Wiśniewski in [BW07]. The first result of Buczyńska and Wiśniewski characterizes the Hilbert polynomial of the algebraic variety associated with the Jukes-Cantor binary model on a tree. Specifically, they showed that this polynomial depends only on the number of leaves of the trivalent tree and not on its topological structure. Their proof relies on deformation theory. In joint work with Haase and Paffenholz, we give a simple combinatorial proof of this statement in Chapter 2:

Main Result 1. *There is a combinatorial proof using piecewise affine unimodular maps that the Hilbert polynomial of the Jukes-Cantor binary model does not depend on the shape of the tree.*

In Chapter 3, we show that analogous statement is not true for the Kimura 3-parameter model, which is the group-based model with the underlying group $\mathbb{Z}_2 \times \mathbb{Z}_2$:

Main Result 2 ([Kub12], Proposition 1)**.** *The Hilbert polynomial of the Kimura 3-parameter model depends on the shape of the tree.*

This result appeared in [Kub12]. In [DM12], Donten-Bury and Michałek showed for several other group-based models that the Hilbert polynomial depends on the shape of the tree.

The second result of Buczyńska and Wiśniewski states that the algebraic variety associated with the Jukes-Cantor binary model on a trivalent tree is normal. Thus the corresponding affine semigroup is generated in degree one [BW07]. Buczyńska introduced the phylogenetic semigroups on trivalent graphs as a generalization of the affine semigroups associated with the Jukes-Cantor binary model on trees [Buc12].

In joint work with Buczyńska, Buczyński, and Michałek [BBKM11], we defined the phylogenetic semigroups on arbitrary graphs and studied the maximal degree of the minimal generating set of the phylogenetic semigroup on a graph with first Betti number g. We showed that $g+1$ is an upper bound for this degree [BBKM11, Mic12]. In Chapter 4, we present the part of [BBKM11] where we study lower bounds for this degree:

Main Result 3 ([BBKM11], Example 4.9)**.** *For g even, there is a graph with first Betti number g such that the maximal degree of the minimal generating set of its phylogenetic semigroup is $g+1$. For g odd, there is a graph with first Betti number g such that this maximal degree is g.*

The minimal generating sets of phylogenetic semigroups have been described for trivalent trees [BW07] and for the trivalent graphs with first Betti number 1 [Buc12]. In Chapter 5, we extend these results in several ways. We characterize the minimal generators of degree $d \leq 2$ of the phylogenetic semigroup on any trivalent graph. Moreover, for any graph with first Betti number $g \leq 1$ and for any trivalent graph with first Betti number 2 we describe the minimal generating set of its phylogenetic semigroup.

Based on the work of Sturmfels and Xu [SX10], Manon showed that the semigroup algebras of phylogenetic semigroups are toric degenerations of the $\mathrm{SL}_2(\mathbb{C})$ conformal block algebras [Man09]. Moreover, in [Man12a] he showed that semigroup algebras of rank two graded Berenstein-Zelevinsky triangles are toric degenerations of $\mathrm{SL}_3(\mathbb{C})$ conformal block algebras.

It follows from this result of Manon that the Hilbert polynomial of the semigroup of rank two graded BZ triangles on a trivalent tree does not depend on the shape of the tree. This generalizes the result of Buczyńska and Wiśniewski that the Hilbert polynomial of the Jukes-Cantor binary model on a trivalent tree does not depend on the shape of the tree, which was not generalizable to other group-based models [Kub12, DM12].

Motivated by these results we ask how group-based models and BZ triangles are related to each other. In Chapter 6, we establish a connection between semigroups associated with the group-based model with the underlying group $\mathbb{Z}_{r+1}$ and rank r BZ triangles:

Main Result 4. *A semigroup associated with the group-based model with the underlying group $\mathbb{Z}_{r+1}$ is included in the projection of the semigroup of rank r BZ triangles to highest weights. For $r = 1, 2$, the equality holds.*

This theorem is a part of joint work with Christoper Manon.

Chapter 1

Preliminaries

This is an introductory chapter. We will cover basic topics that will be used throughout the dissertation. In Section 1.1, we will explain our notation. In Section 1.2, we will introduce lattice polytopes and affine semigroups. In Section 1.3, we will recall the basics about toric varieties, and discuss the correspondence between lattice polytopes and toric varieties. Section 1.4 contains an introduction to phylogenetic algebraic geometry. Finally, we will cover toric fiber products in Section 1.5.

1.1 Notation

For $n \in \mathbb{N}$, we denote $[n] = \{1, 2, \dots, n\}$. Let $u = (u_1, \dots, u_d) \in \mathbb{Z}^d$. We denote by x^u the monomial $x_1^{u_1} \cdot \dots \cdot x_d^{u_d}$. Let $\mathcal{A} = \{a_1 \dots, a_n\} \subset \mathbb{R}^d$ be a set of real vectors. We denote by $\mathbb{N}\mathcal{A} = \{\sum n_i a_i : n_i \in \mathbb{N}\}$ the affine semigroup generated by $\mathcal{A}$, by $\mathbb{Z}\mathcal{A} = \{\sum n_i a_i : n_i \in \mathbb{Z}\}$ the lattice generated by $\mathcal{A}$, by $\operatorname{conv}(\mathcal{A}) = \{\sum \lambda_i a_i : 0 \le \lambda_i \le 1, \sum \lambda_i = 1\}$ the convex hull of $\mathcal{A}$, and by $\operatorname{cone}(\mathcal{A}) = \{\sum \lambda_i a_i : \lambda_i \ge 0\}$ the cone generated by $\mathcal{A}$.

Let G be a graph. The valency or degree of a vertex is the number of edges attached to it (a loop counts twice). A graph is trivalent, if all its vertices have degree one or three. Degree one vertices are called leaves, edges attached to them are called leaf edges. Vertices that are not leaves are called inner nodes, and edges that are not leaf edges are called inner edges. We denote vertices by V, leaves by L, inner nodes by I, and edges by E. Where necessary, we also use $V(G), L(G), I(G)$, and $E(G)$. A claw tree is a tree with one inner node. The claw tree with three leaves is called tripod. We denote the disjoint sum of graphs G_1 and G_2 by $G_1 \sqcup G_2$. We denote by G^e the graph obtained from G by cutting an internal edge e. More specifically, cutting an internal edge e means replacing e by two leaf edges e_1 and e_2 where $\partial_1(e_1) = \partial_1(e)$ and $\partial_1(e_2) = \partial_2(e)$. Here $\partial_1(e), \partial_2(e)$ denote endpoints of an edge e. Let G_1 and G_2 be graphs with distinguished leaves l_1 and l_2, respectively. We denote by $G_1 \star G_2$ their graft, that is the graph obtained from G_1 and G_2 by removing leaves l_1, l_2, and identifying corresponding leaf edges.

1.2 Lattice Polytopes and Affine Semigroups

In this section, we will cover basics about lattice polytopes and affine semigroups. We assume some familiarity with polyhedra, see for example [Zie95, Grü03]. Definitions in this section are based on [Zie95, MS05, CLS11, Pie11].

Definition 1.1. A *lattice* L is a free abelian group in $\mathbb{R}^d$. A *lattice polytope* $P \subset \mathbb{R}^d$ *with respect to a lattice* L is a polytope whose vertices lie in a lattice L. If there is no confusion about the lattice, we often omit "with respect to a lattice L". *Lattice points* of a lattice polytope P are the elements of $P \cap L$.

One typically considers lattice polytopes with respect to the standard lattice $\mathbb{Z}^d$ or the lattice generated by the vertices of the polytope.

Definition 1.2. A *subdivision* S of a polytope $P \subset \mathbb{R}^d$ is a finite collection of polytopes such that

1. the union $\cup_{Q \in S} Q$ of polytopes in S is P,
2. if $Q \in S$, then all the faces of Q are also in S,
3. the intersection $Q_1 \cap Q_2 \in S$ of two polytopes $Q_1, Q_2 \in S$ is a face of both of Q_1 and of Q_2.

A subdivision is a *triangulation* if all the polytopes in S are simplices.

Let $\mathcal{A} = \{a_1, \ldots, a_n\} \subset P$ be a point configuration containing vertices of P, and ω a vector in $\mathbb{R}^n$. The lower hull of $\operatorname{conv}\{(a_1, \omega_1), \ldots, (a_n, \omega_n)\} \subset \mathbb{R}^{d+1}$ gives a subdivision S_ω of P. More specifically, $\operatorname{conv}\{a_{i_1}, \ldots, a_{i_k}\} \in S_\omega$ if and only if $\operatorname{conv}\{(a_{i_1}, \omega_{i_1}), \ldots, (a_{i_k}, \omega_{i_k})\}$ is a face of the lower hull. A subdivision that can be constructed in such a way is called a *regular subdivision of* P. When we want to give priority to the point configuration $\mathcal{A}$, then we say a regular subdivision of $\mathcal{A}$. A regular subdivision that is a triangulation is called a *regular triangulation*.

Let $\pi : \mathbb{R}^d \to \mathbb{R}^{d'}$ be a projection map, and S' a subdivision of $\pi(P)$. Intersecting $\pi^{-1}(Q)$ with P for each $Q \in S'$ gives the *pullback subdivision* $\pi^* S'$ of P.

A lattice simplex $\operatorname{conv}\{v_0, \ldots, v_d\} \subset \mathbb{R}^d$ is *unimodular*, if $|\det(v_1 - v_0, \ldots, v_d - v_0)| = 1$. A triangulation by unimodular simplices is called a *unimodular triangulation*.

Sometimes we denote a subdivision S of a polytope P by $\cup_{i=1}^m P_i$ where $P_1, \ldots, P_m$ are the maximal dimensional polytopes in the subdivision,.

Definition 1.3. For $k \in \mathbb{N}$, the k^{th} *dilation* of a lattice polytope P is the lattice polytope

$$kP = \{kx : x \in P\}.$$

Definition 1.4. A lattice polytope P is *normal* if

$$\underbrace{P \cap L + \ldots + P \cap L}_{k \text{ times}} = kP \cap L$$

for all $k \in \mathbb{N}$.

The inclusion $\subseteq$ always holds. Thus normality means that all lattice points of kP are generated by lattice points of P.

Definition 1.5. The function

$$\mathrm{ehr}_P(k) = |kP \cap L|$$

taking each $k \in \mathbb{N}$ to the number of the lattice points in kP is the *Ehrhart function of* P.

Theorem 1.6 ([MS05], Theorem 12.2)**.** *The function* $\mathrm{ehr}_P(k) : \mathbb{N} \to \mathbb{N}$ *is a polynomial of degree equal to the dimension of* P*, named the Ehrhart polynomial of* P*.*

Besides dimension, one can read other information about a lattice polytope from its Ehrhart polynomial. For example, the leading coefficient of this polynomial is equal to the volume of the lattice polytope.

Example 1.7. The Ehrhart polynomial of

$$P = \mathrm{conv}\{(0,0,0),(1,1,0),(1,0,1),(0,1,1)\}$$

with respect to the standard lattice $\mathbb{Z}^3$ is

$$\mathrm{ehr}_P(k) = \frac{1}{3}k^3 + k^2 + \frac{5}{3}k + 1,$$

and with respect to the lattice $\{x \in \mathbb{Z}^3 : \sum_{i=1}^3 x_i \text{ is even}\}$ generated by the vertices of P is

$$\mathrm{ehr}_P(k) = \frac{1}{6}k^3 + k^2 + \frac{11}{6}k + 1.$$

Definition 1.8. A function

$$\begin{aligned} \phi : \mathbb{R}^d &\to \mathbb{R}^d \\ x &\mapsto Ax + b \end{aligned}$$

with $A \in \mathbb{Z}^{d\times d}$, $|\det(A)| = 1$, and $b \in \mathbb{Z}^d$ is *affine unimodular*.

Lemma 1.9. *Let* $P \subset \mathbb{R}^d$ *be a lattice polytope and* $\phi : \mathbb{R}^d \to \mathbb{R}^d$ *an affine unimodular map. Then*

$$\mathrm{ehr}_P(k) = \mathrm{ehr}_{\phi(P)}(k).$$

Corollary 1.10 ([Kan98], Proposition 5)**.** *Let* $P, Q \subset \mathbb{R}^d$ *be lattice polytopes. If there are subdivisions* $\cup_{i=1}^m P_i$*,* $\cup_{i=1}^m Q_i$*, and a homeomorphism* $\phi : P \to Q$ *such that*

1. $\phi(P_i) = Q_i$ *for* $i = 1, \ldots, m$*,*

2. *the map* ϕ *is affine unimodular on each* P_i*,*

then $\mathrm{ehr}_P(k)$=$\mathrm{ehr}_Q(k)$*.*

Definition 1.11. A *semigroup* is a set S with an associative binary operation and an identity element. A *semigroup homomorphism* is a function between two semigroups that preserves the binary operation and the identity element. The semigroup S is an *affine semigroup*, if it is finitely generated and can be embedded in a lattice, i.e. $S \cong \mathbb{N}\mathcal{A}$ where $\mathcal{A} = \{a_1, \ldots, a_n\} \subset L$. If there exists a vector $\omega \in \mathbb{R}^d$ such that $a_i \cdot \omega \in \mathbb{N}$ for $i = 1, \ldots, n$, then we say that S is $\mathbb{Z}$*-graded* with $\deg(a_i) = a_i \cdot \omega$ for $i = 1, \ldots, n$.

Remark. A semigroup is often defined as a set with an associative binary operation, and a semigroup with an identity element is called a *monoid*. We stick with the notation in the field of combinatorial commutative algebra where an identity element is required from a semigroup.

Example 1.12. Let $P \subset \mathbb{R}^d$ be a lattice polytope with respect to a lattice $L \subset \mathbb{R}^d$. Let $S = \operatorname{cone}(P \times \{1\}) \cap (L \times \{1\})$. By Gordan's Lemma, S has a finite generating set, hence is an affine semigroup. We say that S is the affine semigroup associated with P. The affine semigroup S is *normal* if and only if P is normal. We usually consider S together with the $\mathbb{Z}$-grading induced by the functional $\omega = \{0, \ldots, 0, 1\} \in \mathbb{R}^{d+1}$, i.e. the elements of $(P \times \{1\}) \cap (L \times \{1\})$ have degree one. If the affine semigroup S is normal then it is generated by degree one elements.

1.3 Toric Varieties

Toric geometry is a part of algebraic geometry that can be studied using combinatorial tools. More specifically, there is a well-known correspondence between toric varieties and lattice polytopes. This correspondence is consistent with many properties of toric varieties and lattice polytopes such as dimension, normality, smoothness etc. As a result, questions about toric varieties can frequently be translated to the language of lattice polytopes, and solved using combinatorial methods. Toric varieties are also often used for testing theories in algebraic geometry.

In this section, we will introduce the basics of toric geometry, and then discuss the aforementioned correspondence between toric varieties and lattice polytopes. Standard references on toric geometry are [Oda88, Ful93, Stu96, CLS11]. All definitions in this section are taken almost directly from [Stu96].

Let $\mathcal{A} = \{a_1, \ldots, a_n\}$ be a list of vectors in $\mathbb{Z}^d$. Let π be the semigroup homomorphism

$$\begin{aligned} \pi : \mathbb{N}^n &\to \mathbb{Z}^d \\ u = (u_1, \ldots, u_n) &\mapsto u_1 a_1 + \ldots + u_n a_n. \end{aligned}$$

The image of π is the semigroup $\mathbb{N}\mathcal{A}$. The map π lifts to a semigroup algebra homomorphism

$$\begin{aligned} \hat{\pi} : \mathbb{C}[x_1, \ldots, x_n] &\to \mathbb{C}[t_1^{\pm 1}, \ldots, t_d^{\pm 1}] \\ x_i &\mapsto t^{a_i}. \end{aligned}$$

Definition 1.13. A *toric ideal* is the kernel of $\hat{\pi}$ for some $\mathcal{A}$. It is denoted by $I_{\mathcal{A}}$.

Definition 1.14. An *affine toric variety* is the zero set of a toric ideal $I_{\mathcal{A}}$ in $\mathbb{C}^n$

$$\{x \in \mathbb{C}^n : f(x) = 0 \quad \forall f \in I_{\mathcal{A}}\}.$$

It is denoted by $Y_{\mathcal{A}}$. A *projective toric variety* is the zero set of a homogeneous toric ideal $I_{\mathcal{A}}$ in $\mathbb{P}^{n-1}(\mathbb{C})$. It is denoted by $X_{\mathcal{A}}$.

The varieties $X_{\mathcal{A}}$ and $Y_{\mathcal{A}}$ contain the torus $(t^{a_1}, \dots, t^{a_n})$ with $t \in (\mathbb{C}^*)^d$ as a Zariski open subset. In general, one could define a toric variety as an irreducible variety containing a torus as a Zariski open subset such that the action of the torus on itself extends to an action on the variety [CLS11, Definition 3.1.1]. However, in this dissertation we assume that toric varieties are embedded as in Definition 1.14. Moreover, in contrast to [Ful93] we do not require toric varieties to be normal.

Every vector $u \in \mathbb{Z}^n$ can be written as $u^+ - u^-$ where u^+ is the non-negative and u^- is the negative support of u. Let $\ker(\pi)$ be the sublattice of $\mathbb{Z}^n$ consisting of all vectors u with $\pi(u^+) = \pi(u^-)$.

Lemma 1.15 ([Stu96], Corollary 4.3)**.** $I_{\mathcal{A}} =< x^{u^+} - x^{u^-} : u \in \ker(\pi) >$.

Lemma 1.16 ([CLS11], Proposition 1.1.11)**.** *An ideal $I \subseteq \mathbb{C}[x_1, \dots, x_n]$ is toric if and only if it is prime and generated by binomials.*

Now we will study the correspondence between projective toric varieties and lattice polytopes, their Hilbert and Ehrhart polynomials, initial ideals and regular triangulations.

Lemma 1.17 ([Stu96], Lemma 4.14)**.** *The ideal $I_{\mathcal{A}}$ is homogeneous if and only if there exists a vector $\omega \in \mathbb{Q}^d$ such that $a_i \cdot \omega = 1$ for $i = 1, \dots, n$.*

By the previous lemma, if $I_{\mathcal{A}}$ is homogeneous then the elements of $\mathcal{A}$ lie on an affine hyperplane of $\mathbb{R}^d$. Assuming this is the case, define the polytope $P = \operatorname{conv}(\mathcal{A})$. It is a lattice polytope with respect to the lattice $\mathbb{Z}\mathcal{A}$.

Definition 1.18. The *Hilbert function* of $X_{\mathcal{A}}$ is

$$\operatorname{Hilb}_{\mathcal{A}}(k) = |\{a_{i_1} + \ldots + a_{i_k} : a_{i_1}, \dots, a_{i_k} \in \mathcal{A}\}|, \quad k \geq 0.$$

There exists a polynomial $\mathrm{h}_{\mathcal{A}}(k)$ such that $\mathrm{h}_{\mathcal{A}}(k) = \operatorname{Hilb}_{\mathcal{A}}(k)$ for $k \gg 0$. It is called the *Hilbert polynomial* of $X_{\mathcal{A}}$.

Hilbert polynomials are important invariants of projective varieties. One can read the degree and dimension of a projective variety from its Hilbert polynomial, see [Har77].

Instead of defining normality for projective varieties, we will use [CLS11, Proposition 2.2.18, Definition 2.3.14, Theorem 2.4.1] to state a modified version of [Stu96, Theorem 13.11] that is sufficient for our purposes.

Theorem 1.19 ([Stu96], Theorem 13.11)**.** *If P is normal and $\mathcal{A} = P \cap \mathbb{Z}\mathcal{A}$, then the Hilbert polynomial $\mathrm{h}_{\mathcal{A}}$ and the Ehrhart polynomial ehr_P are equal.*

Definition 1.20. A total order $\prec$ on $\mathbb{N}^n$ is a *term order* if 0 is the unique minimal element and $a \prec b$ implies $a + c \prec b + c$ for all $a, b, c \in \mathbb{N}^n$. Fix a term order $\prec$. For a polynomial $f = \sum c_i x^{a^i}$, the *initial monomial* $\mathrm{in}_\prec(f)$ is $c_i x^{a_i}$ with a_i maximal with respect to $\prec$. The *initial ideal* of an ideal I with respect to $\prec$ is

$$\mathrm{in}_\prec(I) = < \mathrm{in}_\prec(f) : f \in I > .$$

The *initial complex* $\Delta_\prec(I)$ of I with respect to $\prec$ is the simplicial complex on the vertex set $\{1, \ldots, n\}$ with $F \subseteq \{1, \ldots, n\}$ as a face of $\Delta_\prec(I)$ if there is no polynomial $f \in I$ whose initial monomial $\mathrm{in}_\prec(f)$ has support F.

Fix $\omega = (\omega_1, \ldots \omega_n) \in \mathbb{R}^n$. For a polynomial $f = \sum c_i x^{a^i}$, the *initial form* $\mathrm{in}_\omega(f)$ is the sum of $c_i x^{a_i}$ with $\omega \cdot a_i$ maximal. The *initial ideal* of an ideal I with respect to ω is

$$\mathrm{in}_\omega(I) = < \mathrm{in}_\omega(f) : f \in I > .$$

Proposition 1.21 ([Stu96], Proposition 1.11)**.** *For any term order $\prec$ and any ideal $I \in \mathbb{C}[x_1, \ldots, x_n]$, there exists a non-negative integer vector $\omega \in \mathbb{N}^n$ such that $\mathrm{in}_\omega(I) = \mathrm{in}_\prec(I)$.*

Theorem 1.22 ([Stu96], Theorem 8.3)**.** *The regular triangulations of $\mathcal{A}$ are the initial complexes of the toric ideal $I_\mathcal{A}$. More precisely, if $\omega \in \mathbb{R}^n$ represents $\prec$ for $I_\mathcal{A}$, then $\Delta_\prec(I_\mathcal{A}) = S_\omega$.*

Lemma 1.23 ([Stu96], Corollary 8.9)**.** *The initial ideal $\mathrm{in}_\prec(I_\mathcal{A})$ is square-free if and only if the corresponding regular triangulation of $\mathcal{A}$ is unimodular.*

Example 1.24. Let

$$\begin{aligned}\mathcal{A} =&((0,0,0,0,0),(1,1,1,1,0),(1,1,0,0,0),(0,0,1,1,0),\\ &(1,0,1,0,1),(0,1,0,1,1),(1,0,0,1,1),(0,1,1,0,1)).\end{aligned}$$

Then

$$I_\mathcal{A} = < x_{00000}x_{11110} - x_{11000}x_{00110}, x_{10101}x_{01011} - x_{10011}x_{01101} > .$$

The polytope $P = \mathrm{conv}(\mathcal{A})$ is normal with respect to the lattice $\mathbb{Z}\mathcal{A}$ and $\mathcal{A} = P \cap \mathbb{Z}\mathcal{A}$. Hence, the Hilbert polynomial of $X_\mathcal{A}$ and the Ehrhart polynomial of P are equal.

1.4 Phylogenetic Algebraic Geometry

Phylogenetic algebraic geometry studies algebraic varieties associated with statistical models on phylogenetic trees. A phylogenetic tree is a tree of species that describes evolutionary progress based on genetic information, as illustrated in Figure 1.1. In this section, we will explain how to obtain an algebraic variety associated with a statistical model on a phylogenetic tree. Of special interest will be group-based models that give toric varieties. Our discussion is based on [ERSS05, SS05b, Sul07].

Let T be a rooted tree with n leaves. Associate with each vertex a random variable with k possible states. Denote the distribution of the random variable at the root by

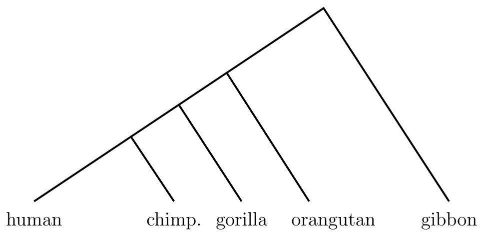


Figure 1.1: A phylogenetic tree

$\pi = (\pi_1, \ldots, \pi_k)$. Associate with each edge e a $k \times k$ transition matrix M_e. The $(i,j)^{\text{th}}$ entry of M_e denotes the probability that the i^{th} state transforms to the j^{th} state along the edge e. The entries of π and M_e are called model parameters. There are $N = k + |E|k^2$ of them. Specifying a subset $P \subseteq \mathbb{R}^N$ of biologically meaningful model parameters means choosing a *statistical model*. The subset P is usually given by polynomial equations and inequalities.

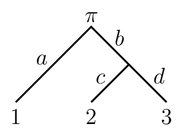
Random variables at leaves are observed variables. There are k^n possibilities for making an observation at n leaves simultaneously. The probability of making a particular observation σ is given by a polynomial ϕ_σ. Polynomials ϕ_σ define a function

$$\phi : \mathbb{R}^N \to \mathbb{R}^{k^n}$$

from the space of model parameters to the space of joint observations.

In phylogenetic algebraic geometry, conditions on the model are weakened. The assumption that the model parameters are non-negative reals that sum up to one is dropped. Instead, one considers the subset $P \subseteq \mathbb{C}^N$ that is given by the polynomial equations that defined the particular model. The central object of study in phylogenetic algebraic geometry is the Zariski closure of $\phi(P)$.

Example 1.25 ([ERSS05], Section 2)**.** Let T be a rooted tree with each vertex corresponding to a random variable with two possible states zero and one.



Let $\pi = (\pi_0, \pi_1)$ denote the root distribution and

$$M_a = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix} \qquad M_b = \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \qquad M_c = \begin{pmatrix} c_{00} & c_{01} \\ c_{10} & c_{11} \end{pmatrix} \qquad M_d = \begin{pmatrix} d_{00} & d_{01} \\ d_{10} & d_{11} \end{pmatrix}$$

the edge transition matrices representing the probabilities of transition between the states. Then the probability of observing the letter i at the leaf 1, the letter j at the leaf 2, and the letter k at the leaf 3 is

$$\phi_{ijk} = \pi_0 a_{0i} b_{00} c_{0j} d_{0k} + \pi_0 a_{0i} b_{01} c_{1j} d_{1k} + \pi_1 a_{1i} b_{10} c_{0j} d_{0k} + \pi_1 a_{1i} b_{11} c_{1j} d_{1k}.$$

Eight polynomials Φ_{ijk} give the map

$$\phi : \mathbb{C}^{18} \to \mathbb{C}^8.$$

Fixing a parameter space $P \subseteq \mathbb{C}^{18}$ specifies the model. The object of interest is the Zariski closure of $\phi(P)$.

In this dissertation, we are interested in group-based models.

Definition 1.26. Let G be a finite additive abelian group. If the k states correspond to the elements of G and the matrices M_e are invariant under the action of G, i.e. for all $h, i, j \in G$, the matrix entry corresponding to (i, j) equals the matrix entry corresponding to $(h + i, h + j)$, then the associated statistical model is called a *group-based model*.

Example 1.27. Group-based models used in computational biology are Jukes-Cantor and Kimura models. The Jukes-Cantor binary model [JC69], also known as the Cavender-Farris-Neyman or just Neyman model [Ney71, Far73, Cav78], is a group-based model with the underlying group $\mathbb{Z}_2$. Transition matrices are of the form

$$M_e = \begin{pmatrix} a & b \\ b & a \end{pmatrix}.$$

The Kimura 3-parameter model [Kim81] is a group-based model with the underlying group $\mathbb{Z}_2 \times \mathbb{Z}_2$. Transition matrices are of the form

$$M_e = \begin{pmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{pmatrix}.$$

It was shown by Evans and Speed that the algebraic variety associated with the Kimura 3-parameter model on a tree is toric after the change of coordinates given by the discrete Fourier transform [ES93]. Székely, Steel, and Erdös extended this approach to group-based models [SSE93] and Michałek to an even larger family of G-models [Mic11]. We will not explain this change of coordinates here as it is not important for further understanding, see [SS05b, Section 2] for a nice exposition. Instead, we will directly define toric varieties associated with group-based models after applying the discrete Fourier transform as in [SS05b, Section 3] and [Sul07, Section 3.4].

We add an extra edge at the root of T to achieve a tree with $n + 1$ leaves. We denote the new tree also by T. Label the new leaf by $n + 1$ and other leaves by $1, \dots, n$. Direct the edges away from the root. A leaf l is a descendant of an edge e if there is a directed path from e to l. Denote by $\mathrm{de}(e)$ the set of all descendants of the edge e.

Let G be a finite additive abelian group. For a sequence $g_1, \dots, g_n$ in G, we define

$$g_e = \sum_{i \in \mathrm{de}(e)} g_i$$

where e is an edge of T. Let

$$\mathbb{C}[x] = \mathbb{C}[x_{g_1,\dots,g_n} : g_i \in G] \text{ and } \mathbb{C}[t] = \mathbb{C}[t_h^{(e)} : e \in E, h \in G],$$

and consider the ring homomorphism

$$\begin{aligned} \phi_{G,T} : \mathbb{C}[x] &\to \mathbb{C}[t] \\ x_{g_1,\dots,g_n} &\mapsto \prod_{e\in E} t_{g_e}^{(e)}. \end{aligned}$$

Definition 1.28. The ideal $I_{G,T} = \ker(\phi_{G,T})$ is the ideal of the group-based model with a group G and a tree T.

This is a homogeneous toric ideal. By the discussion after Lemma 1.17, we can define the associated lattice polytope.

Definition 1.29. The lattice polytope of the group-based model with a group G and a tree T is

$$P_{G,T} = \operatorname{conv}\{x \in \{0,1\}^{E\times G} : \exists g_1,\dots,g_n \in G \text{ such that, } \forall e \in E \text{ and } \forall h \in G,$$

$$x_h^{(e)} = 1 \text{ if } h = \sum_{i\in \operatorname{de}(e)} g_i \text{ and } x_h^{(e)} = 0 \text{ otherwise}\}$$

with respect to the lattice generated by its vertices.

In practice, the construction of the polytope $P_{G,T}$ works as follows. Label the edges of T with elements of G such that at each inner vertex the label on the incoming edge equals the sum of the labels on the outgoing edges. Then replace group elements by unit vectors labeled by these group elements. Finally, write these $|E|$ unit vectors in $\mathbb{R}^G$ as one vector in $\mathbb{R}^{E\times G}$. The polytope P_T is the convex hull of vectors corresponding to all such labelings of the edges of T.

The lattice polytope $P_{G,T}$ lives in the linear subspace of $\mathbb{R}^{E\times|G|}$ defined by $\sum_{h\in G} x_h^{(e)} = 1$ for all edges $e \in E$. Hence, forgetting the coordinate $x_0^{(e)}$ for all $e \in E$ gives a lattice polytope lattice equivalent to $P_{G,T}$. We often consider this projection of $P_{G,T}$, and denote it also by $P_{G,T}$.

Remark. If it is clear from the context which abelian group G is implied, then we often write I_T, P_T, and L_T instead of $I_{G,T}, P_{G,T}$, and $L_{G,T}$.

Example 1.30 ([BW07], Definition 2.9)**.** The lattice polytope of the Jukes-Cantor binary model and a trivalent tree T is

$$P_{\mathbb{Z}_2,T} = \operatorname{conv}\{x \in \{0,1\}^E : \sum_{e\ni v} x_e \in 2\mathbb{Z} \text{ for every } v \in I\}$$

with respect to the lattice

$$L_{\mathbb{Z}_2,T} = \{x \in \mathbb{Z}^E : \sum_{e\ni v} x_e \in 2\mathbb{Z} \text{ for every } v \in I\}.$$

The polytope in Example 1.7 is the lattice polytope of the Jukes-Cantor binary model on the tripod. The polytope in Example 1.24 is the lattice polytope of the Jukes-Cantor binary model on the trivalent 4-leaf tree.

1.5 Toric Fiber Products

The toric fiber product produces from two multigraded homogeneous ideals another multigraded homogeneous ideal. This construction generalizes the Segre embedding of projective spaces. Instead of studying a property on the toric fiber product, one can often study it on the original ideals. Generating sets, Gröbner bases and Hilbert functions provide examples of properties that can be studied in such a way.

The use of the toric fiber product has been especially successful in algebraic statistics: Original ideals correspond to graphs or simplicial complexes, and the toric fiber product corresponds to the graph or simplicial complex obtained by gluing the original structures. For example, Hoşten and Sullivant used the toric fiber product for hierarchical models [HS02], Dobra and Sullivant for k-way tables [DS04], Sturmfels and Sullivant for group-based models [SS05b]. Formally the notion was defined by Sullivant [Sul07], and was further explored by Engström, Kahle, and Sullivant [EKS11]. In this section, we define the toric fiber product of ideals and vector configurations as in [Sul07] and [EKS11], respectively, and then extend the latter definition to lattice polytopes.

Definition 1.31. Let r be a positive integer and s, t vectors of positive integers of length r. Let

$$\mathbb{C}[x] = \mathbb{C}[x_j^i : i \in [r], j \in [s_i]]$$

and

$$\mathbb{C}[y] = \mathbb{C}[y_k^i : i \in [r], k \in [t_i]]$$

be polynomial rings together with a multigrading

$$\deg(x_j^i) = \deg(y_k^i) = a^i \in \mathbb{Z}^d.$$

Assume that there is $\omega \in \mathbb{R}^d$ such that $a^i \cdot \omega = 1$ for $i = 1, \ldots, r$. This means that ideals that are homogeneous with respect to this multigrading are also homogeneous with respect to the standard grading. Let $\mathcal{A}$ denote $\{a^1, \ldots, a^r\}$.

Let I and J be homogeneous ideals with respect to this multigrading in $\mathbb{C}[x]$ and $\mathbb{C}[y]$, respectively. Therefore $R = \mathbb{C}[x]/I$ and $S = \mathbb{C}[y]/J$ are also multigraded rings. Let

$$\mathbb{C}[z] = \mathbb{C}[z_{jk}^i : i \in [r], j \in [s_i], k \in [t_j]]$$

be a polynomial ring. Define a map $\phi_{I,J}$ from $\mathbb{C}[z]$ to $R \otimes S$ by

$$z_{jk}^i \mapsto x_j^i \otimes y_k^i.$$

The *toric fiber product of the ideals* I and J is the kernel of the map ϕ

$$I \times_{\mathcal{A}} J = \ker(\phi_{I,J}).$$

Example 1.32 ([Sul07], Example 1.2)**.** If $r = 1$ and $I = J = 0$, then

$$I \times_{\mathcal{A}} J =< z_{j_1k_1}z_{j_2k_2} - z_{j_1k_2}z_{j_2k_1} : j_1, j_2 \in [s], k_1, k_2 \in [t] >$$

is the Segre product of $\mathbb{P}^{s-1}$ and $\mathbb{P}^{t-1}$.

Definition 1.33. Let r be a positive integer and s, t vectors of positive integers of length r. Let

$$\mathcal{B} = \{b^i_j : i \in [r], j \in [s_i]\} \subset \mathbb{Z}^{d'}$$

and

$$\mathcal{C} = \{c^i_k : i \in [r], k \in [t_i]\} \subset \mathbb{Z}^{d''}$$

be vector configurations together with linear maps $\pi' : \mathbb{Z}^{d'} \to \mathbb{Z}^d$ and $\pi'' : \mathbb{Z}^{d''} \to \mathbb{Z}^d$ such that

$$\pi'(b^i_j) = \pi''(c^i_k) = a^i \in \mathbb{Z}^d.$$

Let $\mathcal{A}$ denote $\{a^1, \dots, a^r\}$. The *toric fiber product of the vector configurations* $\mathcal{B}$ and $\mathcal{C}$ with respect to $\mathcal{A}$ is

$$\mathcal{B} \times_{\mathcal{A}} \mathcal{C} = \{(b^i_j, c^i_k) \in \mathcal{B} \times \mathcal{C} : i \in [r], j \in [s_i], k \in [t_j]\}.$$

Let $I_{\mathcal{B}}$ and $I_{\mathcal{C}}$ be toric ideals corresponding to the vector configurations $\mathcal{B}$ and $\mathcal{C}$. By [EKS11, Section 2.3],

$$I_{\mathcal{B}} \times_{\mathcal{A}} I_{\mathcal{C}} = I_{\mathcal{B} \times_{\mathcal{A}} \mathcal{C}}. \tag{1.1}$$

Definition 1.34. Let r be a positive integer and s, t vectors of positive integers of length r. Let $P' \subset \mathbb{R}^{d'}, P'' \subset \mathbb{R}^{d''}$ be lattices polytopes with respect to lattices $L' \subset \mathbb{Z}^{d'}, L'' \subset \mathbb{Z}^{d''}$ such that

$$P' \cap L' = \{b^i_j : i \in [r], j \in [s_i]\}$$

and

$$P'' \cap L'' = \{c^i_k : i \in [r], k \in [t_i]\}$$

together with linear maps $\pi' : L' \to \mathbb{Z}^d, \pi'' : L'' \to \mathbb{Z}^d$ such that

$$\pi'(b^i_j) = \pi''(c^i_k) = a^i \in \mathbb{Z}^d.$$

Let $\mathcal{A}$ denote $\{a^1, \dots, a^r\}$. The *toric fiber product of the lattice polytopes* P' and P'' is

$$P' \times_{\mathcal{A}} P'' = \operatorname{conv}\{(P' \cap L') \times_{\mathcal{A}} (P'' \cap L'')\}.$$

It is a lattice polytope with respect to the lattice generated by $(P' \cap L') \times_{\mathcal{A}} (P'' \cap L'')$. By (1.1),

$$I_{P' \cap L'} \times_{\mathcal{A}} I_{P'' \cap L''} = I_{(P' \cap L') \times_{\mathcal{A}} (P'' \cap L'')}.$$

Group-based models provide examples of toric fiber products. Fix a finite additive abelian group G. Let T be a directed tree with an inner edge e. Cutting e induces a decomposition of T as $T^+_e \star T^-_e$. Let $\mathbb{C}[x], \mathbb{C}[x]_+, \mathbb{C}[x]_-$ denote the ambient polynomial rings of $I_{G,T}, I_{G,T^+_e}, I_{G,T^-_e}$, respectively.

Theorem 1.35 ([Sul07], Theorem 3.10)**.** *Let T be a tree with an inner edge e. For each variable $x_{\mathbf{g}}$ in $\mathbb{C}[x], \mathbb{C}[x]_+$, and $\mathbb{C}[x]_-$, let deg$(x_{\mathbf{g}}) = e_{g_e}$, the standard unit vector with label g_e. Let $\mathcal{A} = \{e_h : h \in G\}$. Then*

$$I_{G,T} = I_{G,T_e^+} \times_{\mathcal{A}} I_{G,T_e^-}.$$

Corollary 1.36. *Let T be a tree with an inner edge e. For each lattice point $x_{\mathbf{g}}$ of $P_{G,T}, P_{G,T_e^+}$, and P_{G,T_e^-}, let deg$(x_{\mathbf{g}}) = e_{g_e}$, the standard unit vector with label g_e. Let $\mathcal{A} = \{e_h : h \in G\}$. Then*

$$P_{G,T} = P_{G,T_e^+} \times_{\mathcal{A}} P_{G,T_e^-}.$$

Example 1.37. The polytope in Example 1.24 is the toric fiber product of the polytope in Example 1.7 with itself with respect to the projection onto an edge of the tripod.

Chapter 2

Combinatorial Proof of a Theorem by Buczyńska and Wiśniewski

2.1 Introduction

This chapter is based on discussions with Christian Haase and Andreas Paffenholz.

The Jukes-Cantor binary model is the simplest group-based model with the underlying group $\mathbb{Z}_2$. Algebraic varieties associated with it are well-studied [SS05b, BW07, CP07, DM12]. The Jukes-Cantor binary model turns out to be a very special model having beautiful properties not true or not known for other group-based models. In this chapter, we are interested in one of them.

Theorem 2.1 ([BW07], Theorem 2.24)**.** *The Hilbert polynomial of the algebraic variety associated with the Jukes-Cantor binary model on a trivalent tree depends only on the number of leaves of the tree, and not on its shape.*

Buczyńska generalized this result to the phylogenetic semigroups on trivalent graphs that generalize the Jukes-Cantor binary model on trees [Buc12]. Specifically, she showed that the Hilbert polynomial of the phylogenetic semigroup on a trivalent graph depends only on the first Betti number and the number of leaves of the graph.

In the original proof of Theorem 2.1, Buczyńska and Wiśniewski showed that any two algebraic varieties associated with the Jukes-Cantor binary model on trees with the same number of leaves are deformation equivalent [BW07]. Alternative proofs have been given by Sturmfels and Xu using sagbi degenerations [SX10], and by Ilten using deformations of complexity-one T-varieties [Ilt10]. We will give a purely combinatorial proof using continuous piecewise affine unimodular maps of lattice polytopes. However, also our proof has a geometric meaning. We construct Gröbner degenerations of algebraic varieties associated with the Jukes-Cantor binary model to a common initial scheme.

Given two lattice polytopes $P, Q \in \mathbb{R}^d$ with equal Ehrhart polynomials, it is not known if there always exists a continuous piecewise affine unimodular map $\phi : P \to Q$. Such maps are known between order and chain polytopes [Sta86], and Gelfand-Tsetlin and Feigin-Fourier-Littelmann polytopes [ABS11]. In dimension two, Greenberg showed that there always exists a continuous piecewise affine unimodular map between Ehrhart equivalent lattice polytopes [Gre93]. Kantor conjectured that in higher dimensions such a map does not need to exist [Kan98]. The best result known is by Haase and McAllister [HM08]: They show that two integral polytopes are Ehrhart equivalent if and only if they can be decomposed into open rational polytopes $P_1, P_2, \dots, P_n$ and $Q_1, Q_2, \dots, Q_n$, respectively, such that P_j is equivalent to Q_j via $\mathrm{GL}_d(\mathbb{Z}) \ltimes \mathbb{Q}^d$. This map need not to be continuous.

The situation is different, if instead of looking for piecewise affine unimodular maps, we look for piecewise volume-preserving maps. In [Pak13, Chapter 18], Pak gave a constructive proof showing the existence of a continuous piecewise linear volume-preserving map between any two polytopes of equal volume.

In this chapter, we consider families of lattice polytopes indexed by trivalent trees. We study when is the Ehrhart polynomial of a lattice polytope in such a family independent of the shape of the tree. In Section 2.2, we show how to reduce this question to a single polytope associated with the 4-leaf tree, and give a sufficient condition for the Ehrhart polynomial to be independent of the shape of a tree. In Section 2.3, we apply this condition to the Jukes-Cantor binary model to give a combinatorial proof of Theorem 2.1.

2.2 Families of Lattice Polytopes

For any tree T and an inner edge e of T, denote by T_e^+ and T_e^- the trees obtained from T by cutting the edge e.

Definition 2.2. Let $\{P_T\}$ be a family of lattice polytopes with respect to lattices $\{L_T\}$ indexed by trivalent trees. Assume that

1. for any T, $e \in E$, and a fixed $k \in \mathbb{N}$, there is a linear map $p_{T,e} : L_T \to \mathbb{Z}^k$,
2. for any T and e an inner edge of T, the polytope P_T is the toric fiber product of $P_{T_e^+}$ and $P_{T_e^-}$ with respect to the linear maps $p_{T_e^+,e}$ and $p_{T_e^-,e}$.

Then we say that $\{P_T\}$ is a toric fiber product family of lattice polytopes indexed by trivalent trees.

Example 2.3. Let G be a finite additive abelian group. Then the family $\{P_{G,T}\}$ of lattice polytopes associated with the group-based model with the underlying group G is a toric fiber product family. By Corollary 1.36, the polytope $P_{G,T}$ is the toric fiber product of P_{G,T_e^+} and P_{G,T_e^-} with respect to the projections onto the edge e.

The aim of this section is to give a sufficient condition for the Ehrhart polynomial of a toric fiber product family of lattice polytopes indexed by trivalent trees not to depend on the shape of the tree, but only on the number of leaves. First, we explain how to reduce the question about the invariance of the Ehrhart polynomial to one polytope associated with the trivalent 4-leaf tree instead of considering an infinite number of polytopes.

Remark. There are two reasons why we do not want to restrict ourselves only to group-based models, and instead use the more general Definition 2.2. The Jukes-Cantor binary model seems to be the only group-based model whose Ehrhart polynomial does not depend on the shape of the tree, see [Kub12, DM12]. Thus there is no need for a sufficient condition for other group-based models. However, there is a family of lattice polytopes associated with rank two BZ triangles that is a toric fiber product family and has this property, see [Man12a].

We recall the notion of the mutation equivalence of trivalent trees defined by Buczyńska and Wiśniewski in [BW07]. Let T_0 be the trivalent 4-leaf tree and e its inner edge. There are three non-isomorphic labelings of the leaves of T_0, shown in Figure 2.1. Given four rooted trivalent trees T_i where $i = 1, \ldots, 4$, we can produce three trees by grafting the tree T_i along the i^{th} leaf of the labeled T_0. These three trees need not be different.

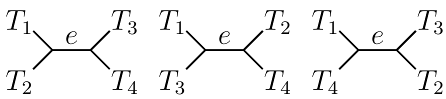


Figure 2.1: Labelings of the trivalent 4-leaf tree

Definition 2.4 ([BW07], Definition 2.17)**.** We say that there exists an elementary mutation along the edge e from one of the above trees to the other two. We say that two trees are mutation equivalent if there exists a sequence of elementary mutations from one to the other.

Lemma 2.5 ([BW07], Lemma 2.18)**.** *Any two trivalent trees with the same number of leaves are mutation equivalent.*

If we are able to show that $\mathrm{ehr}_{P_T}(k) = \mathrm{ehr}_{P_{T'}}(k)$ for any two trivalent trees T and T' that differ by an elementary mutation, then it follows for any two trees with the same number of leaves by applying a sequence of elementary mutations. Hence, we can restrict ourselves to the pairs of trivalent trees that differ by an elementary mutation.

Let T and T' be trivalent trees that differ by an elementary mutation along an edge e. Let T_0 be the trivalent 4-leaf tree with the inner edge e. For $i = 1, \ldots, 4$, let T_i be rooted trivalent trees such that we can produce T and T' by grafting the tree T_i along the i^{th} leaf of a labeled T_0. Denote by p_i and p'_i the projections corresponding to the edges labeled by i in those labelings of the leaves of T_0 that correspond to T and T'.

Lemma 2.6. *Let* $\cup_{j=1}^n P_j$ *and* $\cup_{j=1}^n Q_j$ *be two subdivisions of* P_{T_0} *and* $\phi : P_{T_0} \to P_{T_0}$ *a homeomorphism with*

1. $\phi(P_j) = Q_j$ *for all* j,
2. ϕ *is affine unimodular on each* P_j,

3. $p_i(v) = p'_i(\phi(v))$ *for all lattice points* v *of* P_{T_0} *and* $i = 1, \ldots, 4$.

Then there exist subdivisions $\cup_{j=1}^n \overline{P_j}$ *and* $\cup_{j=1}^n \overline{Q_j}$ *of* P_T *and* $P_{T'}$*, respectively and a homeomorphism* $\overline{\phi} : P_T \to P_{T'}$ *such that*

1. $\overline{\phi}(\overline{P_j}) = \overline{Q_j}$ *for all* j*,*

2. $\overline{\phi}$ *is affine unimodular on each* $\overline{P_j}$*.*

Proof. Polytopes P_T and $P_{T'}$ are toric fiber products of P_{T_i} where $i = 0, \ldots, 4$. Hence, there are projections from P_T and $P_{T'}$ to P_{T_0}. Subdivisions $\cup_{j=1}^n P_j$ and $\cup_{j=1}^n Q_j$ can be pulled back to subdivisions $\cup_{j=1}^n \overline{P_j}$ of P_T and $\cup_{j=1}^n \overline{Q_j}$ of $P_{T'}$. Define $\overline{\phi} : P_T \to P_{T'}$ as follows: $\overline{\phi}|_{P_{T_0}} := \phi$ and $\overline{\phi}|_{P_{T_i}} := \mathrm{id}_{P_{T_i}}$ for $i = 1, \ldots, 4$. The condition $p_i(v) = p'_i(\phi(v))$ ensures that $\overline{\phi}$ is well-defined. □

Corollary 2.7. *If the assumptions of Lemma 2.6 are fulfilled, then* $\mathrm{ehr}_{P_T}(k) = \mathrm{ehr}_{P_{T'}}(k)$*.*

Finally, we describe one case where we can construct a map like in Lemma 2.6. We will use the connection between triangulations of lattice polytopes and initial ideals of corresponding toric ideals.

We fix a labeling of the leaves of T_0. For $i \in \{1, 2, 3, 4\}$, let p_i be the projection onto the edge of T_0 labeled by i in this labeling. Assume that there is a one-to-one correspondence between the lattice points of P_{T_0} and their projections

$$\{(p_1(x), p_2(x), p_3(x), p_4(x)) : x \text{ is a lattice point of } P_{T_0}\}.$$

Moreover, assume that this set is independent of the labeling we fixed.

We fix also a second labeling of the leaves of T_0. For $i \in \{1, 2, 3, 4\}$, let p'_i be the projection onto the edge of T_0 labeled by i in this labeling. By the first assumption, we can replace the subindices of the variables in the coordinate ring associated with P_{T_0} by their projections $(p_1(x), p_2(x), p_3(x), p_4(x))$, i.e. instead of

$$\mathbb{C}[z_x : x \text{ is a lattice point of } P_{T_0}],$$

we can consider

$$\mathbb{C}[z_{p_1(x),p_2(x),p_3(x),p_4(x)} : x \text{ is a lattice point of } P_{T_0}].$$

By the second assumption, the subindices of the variables in the coordinate rings

$$\mathbb{C}[z_{p_1(x),p_2(x),p_3(x),p_4(x)} : x \text{ is a lattice point of } P_{T_0}]$$

and

$$\mathbb{C}[z_{p'_1(x),p'_2(x),p'_3(x),p'_4(x)} : x \text{ is a lattice point of } P_{T_0}]$$

are equal. Denote the toric ideal associated with the lattice polytope P_{T_0} in coordinates $z_{p_1(x),p_2(x),p_3(x),p_4(x)}$ by I_{T_0} and in coordinates $z_{p'_1(x),p'_2(x),p'_3(x),p'_4(x)}$ by I'_{T_0}.

Proposition 2.8. *If there exist term orders $\prec$ and $\prec'$ with $\text{in}_\prec(I_{T_0}) = \text{in}_{\prec'}(I'_{T_0})$, then there is a homeomorphism $\phi : P_{T_0} \to P_{T_0}$ that fulfills the 1. and 3. assumption of Lemma 2.6.*

Proof. Let $\text{conv}\{x_0, \dots, x_d\}$ be a maximal simplex in the triangulation $\Delta_\prec(I_{T_0})$. Define ϕ on $\text{conv}\{x_0, \dots, x_d\}$ as follows: Let $\phi(x_j)$ be the unique lattice point of P_{T_0} with $p'_i(\phi(x_j)) = p_i(x_j)$ for $i \in \{1, \dots, 4\}$. Then $\text{conv}\{\phi(x_0), \dots, \phi(x_d)\}$ is a maximal simplex in the triangulation $\Delta_{\prec'}(I'_{T_0})$, because $\text{in}_\prec(I_{T_0}) = \text{in}_{\prec'}(I'_{T_0})$ and the monomial corresponding to $\text{conv}\{x_0, \dots, x_d\}$ in $\mathbb{C}[z_{p_1(x),p_2(x),p_3(x),p_4(x)} : x \text{ is a lattice point of } P_{T_0}]$ is the same as the monomial corresponding to $\text{conv}\{\phi(x_0), \dots, \phi(x_d)\}$ in $\mathbb{C}[z_{p'_1(x),p'_2(x),p'_3(x),p'_4(x)} : x \text{ is a lattice point of } P_{T_0}]$. The 1. and 3. condition of Lemma 2.6. are fulfilled by the definition of ϕ. $\square$

If ϕ fulfills also the 2. condition of Lemma 2.6, then we get a map like in Lemma 2.6.

Corollary 2.9. *If there exist term orders $\prec$ and $\prec'$ with $\text{in}_\prec(I_{T_0}) = \text{in}_{\prec'}(I'_{T_0})$ square-free, then there is a homeomorphism $\phi : P_{T_0} \to P_{T_0}$ that fulfills the 1., 2., and 3. assumption of Lemma 2.6.*

Proof. Define ϕ as in Proposition 2.8. By Lemma 1.23, the triangulations $\Delta_\prec(I_{T_0})$ and $\Delta_{\prec'}(I'_{T_0})$ are unimodular. Hence, the map ϕ is affine unimodular on each simplex. $\square$

2.3 Jukes-Cantor Binary Model

In this section, we apply Corollary 2.7, Proposition 2.8, and Corollary 2.9 to give a purely combinatorial proof of Theorem 2.1: The Hilbert polynomial of the algebraic variety associated with the Jukes-Cantor binary model on a trivalent tree does not depend on the topology of the tree.

By [BW07], algebraic varieties associated with the Jukes-Cantor model on trivalent trees are normal. By Theorem 1.19, the Hilbert polynomial of the algebraic variety and the Ehrhart polynomial of the lattice polytope associated with the Jukes-Cantor binary model on a trivalent tree are equal. We recall that the lattice polytope associated with the Jukes-Cantor binary model on a trivalent tree T is

$$P_{\mathbb{Z}_2,T} = \text{conv}\{x \in \{0,1\}^E : \sum_{e \ni v} x_e \in 2\mathbb{Z} \text{ for every } v \in I\}.$$

The associated lattice is

$$L_{\mathbb{Z}_2,T} = \{x \in \mathbb{Z}^E : \sum_{e \ni v} x_e \in 2\mathbb{Z} \text{ for every } v \in I\}.$$

In particular,

$$P_{\mathbb{Z}_2,T_0} = \text{conv}\left\{ \begin{array}{cccc} (0,0,0,0,0) & (1,1,1,1,0) & (1,1,0,0,0) & (0,0,1,1,0) \\ (1,0,1,0,1) & (0,1,0,1,1) & (1,0,0,1,1) & (0,1,1,0,1) \end{array} \right\}.$$

Here the first four coordinates of $P_{\mathbb{Z}_2,T_0}$ correspond to the leaf edges of T_0 labeled by $1,\ldots,4$ in the first labeling in Figure 2.1, and the fifth coordinate corresponds to the inner edge.

Consider two different labelings of the leaves of T_0, say the first and the second one in Figure 2.1. The discussion for any other pair of labelings of the leaves of T_0 is analogous. The variables corresponding to the first labeling are

$$z_{0000}, z_{1111}, z_{1100}, z_{0011}, z_{1010}, z_{0101}, z_{1001}, z_{0110},$$

and to the second labeling are

$$z_{0000}, z_{1111}, z_{1010}, z_{0101}, z_{1100}, z_{0011}, z_{1001}, z_{0110}.$$

The ambient coordinate ring is in both cases

$$\mathbb{C}[z_{0000}, z_{1111}, z_{1100}, z_{0011}, z_{1010}, z_{0101}, z_{1001}, z_{0110}].$$

The toric ideals corresponding to the different labelings are

$$\begin{aligned} I_{\mathbb{Z}_2,T_0} &=< z_{0000}z_{1111} - z_{1100}z_{0011}, z_{1010}z_{0101} - z_{1001}z_{0110} >, \\ I'_{\mathbb{Z}_2,T_0} &=< z_{0000}z_{1111} - z_{1010}z_{0101}, z_{1100}z_{0011} - z_{1001}z_{0110} > . \end{aligned}$$

There are two different initial ideals that work for Proposition 2.8. We will explicitly describe them in the next two subsections.

First transformation

Let ω be the weight vector that has 2's corresponding to the variables $z_{1100}, z_{0011}, z_{1010}, z_{0101}$ and 1's corresponding to the rest of the variables. The ideal

$$< z_{1100}z_{0011}, z_{1010}z_{0101} > \tag{2.1}$$

is a common initial ideal of $I_{\mathbb{Z}_2,T_0}$ and $I'_{\mathbb{Z}_2,T_0}$ for any term order that refines the weight order given by ω. The maximal simplices in the corresponding triangulations are

$$\begin{aligned} &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(1,1,0,0,0),(1,0,1,0,1),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(1,1,0,0,0),(0,1,0,1,1),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(0,0,1,1,0),(1,0,1,0,1),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(0,0,1,1,0),(0,1,0,1,1),(1,0,0,1,1),(0,1,1,0,1)\}, \end{aligned}$$

and

$$\begin{aligned} &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(1,0,1,0,1),(1,1,0,0,0),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(1,0,1,0,1),(0,0,1,1,0),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(0,1,0,1,1),(1,1,0,0,0),(1,0,0,1,1),(0,1,1,0,1)\}, \\ &\text{conv}\{(0,0,0,0,0),(1,1,1,1,0),(0,1,0,1,1),(0,0,1,1,0),(1,0,0,1,1),(0,1,1,0,1)\}. \end{aligned}$$

The first triangulation is mapped to the second one by the maps

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & -1 & 0 & 1 \end{pmatrix} x,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & 1 \end{pmatrix} x,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 & 1 \end{pmatrix} x,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 1 & 0 & 1 \end{pmatrix} x.$$

All these matrices have determinant ± 1, and hence are unimodular with respect to the standard lattice $\mathbb{Z}^5$. By Proposition 2.8 and Corollary 2.7, the Ehrhart polynomial of the lattice polytope associated with the Jukes-Cantor binary model and a trivalent tree with respect to the standard lattice depends only on the number of leaves of the tree.

Since the ideal (2.1) is square-free, by Corollary 2.9 and Corollary 2.7 we get the same statement for the lattice generated by the vertices of the polytope. This implies Theorem 2.1 by Buczyńska and Wiśniewski.

Remark. The min-max description of this map is

$$\begin{aligned} x'_1 &= x_1, \\ x'_2 &= x_3, \\ x'_3 &= x_2, \\ x'_4 &= x_4, \\ x'_5 &= x_2 - x_3 + x_5 + \min(x_1 - x_2 + x_3 - x_4, 0) - \min(x_1 + x_2 - x_3 - x_4, 0). \end{aligned}$$

The min-max description can be constructed from the equalities

$$x_1 - x_2 + x_3 - x_4 = 0,$$
$$x_1 + x_2 - x_3 - x_4 = 0.$$

that define the triangulation above.

Second transformation

Let ω be the weight vector that has 2's corresponding to the variables $z_{0000}, z_{1111}, z_{1001}, z_{0110}$ and 1's corresponding to the rest of the variables. The ideal

$$< z_{0000}z_{1111}, z_{1001}z_{0110} > . \tag{2.2}$$

is a common initial ideal of $I_{\mathbb{Z}_2,T_0}$ and $I'_{\mathbb{Z}_2,T_0}$ for any term order that refines the weight order given by ω. Maximal simplices in the corresponding triangulations are

$$\begin{aligned}
&\mathrm{conv}\{(0,0,0,0,0),(1,1,0,0,0),(0,0,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(1,0,0,1,1)\},\\
&\mathrm{conv}\{(0,0,0,0,0),(1,1,0,0,0),(0,0,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(0,1,1,0,1)\},\\
&\mathrm{conv}\{(1,1,1,1,0),(1,1,0,0,0),(0,0,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(1,0,0,1,1)\},\\
&\mathrm{conv}\{(1,1,1,1,0),(1,1,0,0,0),(0,0,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(0,1,1,0,1)\},
\end{aligned}$$

and

$$\begin{aligned}
&\mathrm{conv}\{(0,0,0,0,0),(1,0,1,0,1),(0,1,0,1,1),(1,1,0,0,0),(0,0,1,1,0),(1,0,0,1,1)\},\\
&\mathrm{conv}\{(0,0,0,0,0),(1,0,1,0,1),(0,1,0,1,1),(1,1,0,0,0),(0,0,1,1,0),(0,1,1,0,1)\},\\
&\mathrm{conv}\{(1,1,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(1,1,0,0,0),(0,0,1,1,0),(1,0,0,1,1)\},\\
&\mathrm{conv}\{(1,1,1,1,0),(1,0,1,0,1),(0,1,0,1,1),(1,1,0,0,0),(0,0,1,1,0),(0,1,1,0,1)\}.
\end{aligned}$$

The first triangulation is mapped to the second one by the maps

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & -1 \end{pmatrix} x,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & -1 \end{pmatrix} x,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 & -1 \end{pmatrix} x + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2 \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & -1 & -1 \end{pmatrix} x + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2 \end{pmatrix}.$$

All these matrices have determinant ± 1, and hence are affine unimodular with respect to the standard lattice $\mathbb{Z}^5$. By Proposition 2.8 and Corollary 2.7, the Ehrhart polynomial of the lattice polytope associated with the Jukes-Cantor binary model and a trivalent tree with respect to the standard lattice depends only on the number of leaves of the tree.

Since the ideal (2.2) is square-free, by Corollary 2.9 and Corollary 2.7 we get the same statement for the lattice generated by the vertices of the polytope. This implies Theorem 2.1 by Buczyńska and Wiśniewski.

Remark. The min-max description of this map is

$$\begin{aligned}
x'_1 &= x_1, \\
x'_2 &= x_3, \\
x'_3 &= x_2, \\
x'_4 &= x_4, \\
x'_5 &= x_1 + x_4 - x_5 - \min(x_1 - x_2 - x_3 + x_4, 0) + \min(2 - x_1 - x_2 - x_3 - x_4, 0).
\end{aligned}$$

Phylogenetic semigroups

In this subsection, we will explore the bijections established by the piecewise affine unimodular maps in the previous two subsections. Our goal is to explain how our method gives a combinatorial proof of a result by Buczyńska about the Hilbert functions of the phylogenetic semigroups on trivalent graphs.

Fix two labelings of the leaves of T_0. For $i \in \{1, 2, 3, 4\}$, let p_i, p'_i be the projections onto the edges of T_0 labeled by i in the corresponding labelings. Recall the assumptions of Section 2.2 that there is a one-to-one correspondence between the lattice points of P_{T_0} and their projections

$$\{(p_1(x), p_2(x), p_3(x), p_4(x)) : x \text{ is a lattice point of } P_{T_0}\},$$

and that this set is independent of the labeling we fixed. Hence, there is a natural bijection f from the set

$$\{x \in P_{T_0} \cap L_{T_0} : p_i(x) = u_i \text{ for } i \in \{1, 2, 3, 4\}\}$$

to the set

$$\{x \in P_{T_0} \cap L_{T_0} : p'_i(x) = u_i \text{ for } i \in \{1,2,3,4\}\}$$

for all $u \in \{0,1\}^4$.

By the normality of P_{T_0}, every element x of $kP_{T_0} \cap L_{T_0}$ can be written as $x_1+x_2+\ldots+x_k$ where $x_1, x_2, \ldots, x_k \in P_{T_0} \cap L_{T_0}$. Moreover, for a term order $\prec$ as in Proposition 2.8, we define the canonical representation of x to be the sum $x_1 + x_2 + \ldots + x_k$ such that $x_1 x_2 \ldots x_k \notin \mathrm{in}_\prec(I_{T_0})$. Define $f_k : kP_{T_0} \cap L_{T_0} \to kP_{T_0} \cap L_{T_0}$ by

$$f_k(x) := f(x_1) + f(x_2) + \ldots + f(x_k)$$

where $x_1 + x_2 + \ldots + x_k$ is the canonical representation of x. Since $p_i(x_j) = p'_i(f(x_j))$ for all $i \in \{1,2,3,4\}$ and $j \in \{1,2,\ldots,k\}$ by the definition of f, we have $p_i(x) = p'_i(f_k(x))$ for all $i \in \{1,2,3,4\}$. The map f_k is bijective, because $f(x_1) + f(x_2) + \ldots + f(x_k)$ is the canonical representation of $f_k(x)$ for a term order $\prec'$ as in Proposition 2.8, hence we can define the inverse of f_k. Therefore, the map f_k induces a bijection between the sets

$$\{x \in kP_{T_0} \cap L_{T_0} : p_i(x) = u_i \text{ for } i \in \{1,2,3,4\}\} \tag{2.3}$$

and

$$\{x \in kP_{T_0} \cap L_{T_0} : p'_i(x) = u_i \text{ for } i \in \{1,2,3,4\}\} \tag{2.4}$$

for all $u \in \mathbb{N}^4$ and $k \in \mathbb{N}$.

Let T and T' be trivalent trees that differ by an elementary mutation along an edge e. Let T_0 be the trivalent 4-leaf tree with the inner edge e. For $i = 1, \ldots, 4$, let T_i be rooted trivalent trees such that we can produce T and T' by grafting the tree T_i along the i^{th} leaf of a labeled T_0. Denote by p_i and p'_i the projections corresponding to the edges labeled by i in those labelings of T_0 that correspond to T and T'.

The number of the lattice points in kP_T is

$$\sum_{u \in \mathbb{N}^4} |\{x \in kP_{T_0} \cap L_{T_0} : p_i(x) = u_i \text{ for } i \in \{1,2,3,4\}\}| \prod_{i=1}^{4} |\{x \in kP_{T_i} \cap L_{T_i} : x_i = u_i\}| \tag{2.5}$$

where x_i is the coordinate of $x \in kP_{T_i} \cap L_{T_i}$ that corresponds to the edge of T that is identified with the edge of T_0 labeled by i. We get a similar formula for the number of the lattice points in $kP_{T'}$:

$$\sum_{u \in \mathbb{N}^4} |\{x \in kP_{T_0} \cap L_{T_0} : p'_i(x) = u_i \text{ for } i \in \{1,2,3,4\}\}| \prod_{i=1}^{4} |\{x \in kP_{T_i} \cap L_{T_i} : x_i = u_i\}|. \tag{2.6}$$

Since we have a bijection between the sets (2.3) and (2.4), we get a bijection between the lattice points of kP_T and $kP_{T'}$. By Lemma 2.5, this bijection can be extended to any two trivalent trees with the same number of leaves.

In Chapter 4, we will define the phylogenetic semigroup $\tau(G)$ on a graph G as a generalization of the Jukes-Cantor binary model on trees. Buczyńska proved that similarly to the trees case, the Hilbert function of $\tau(G)$ where G is a trivalent graph depends only on the combinatorial data of G, the first Betti number and the number of leaves of G [Buc12, Theorem 3.5]. Without explicitly defining the phylogenetic semigroup on a graph here, we briefly explain how to use the method in this chapter to give a combinatorial proof of this more general statement of Buczyńska.

Similarly to Definition 2.4 and Lemma 2.5, Buczyńska defined elementary mutations and mutation equivalence for trivalent graphs [Buc12, Definition 2.7] and proved that any two trivalent graphs with the same first Betti number and the same number of leaves are mutation equivalent [Buc12, Lemma 2.10]. Let G and G' be trivalent graphs that differ by an elementary mutation. We can write down formulas for the number of the lattice points in the k^{th} graded piece of $\tau(G)$ and $\tau(G')$ similar to (2.5) and (2.6), respectively, and establish a bijection between the lattice points of the k^{th} graded piece of $\tau(G)$ and $\tau(G')$. By [Buc12, Lemma 2.10], this bijection can be extended to any two trivalent graphs with the same first Betti number and the same number of leaves.

Chapter 3

Hilbert Polynomial of the Kimura 3-Parameter Model

3.1 Introduction

In the last chapter, we gave a combinatorial proof to the theorem by Buczyńska and Wiśniewski saying that the Hilbert polynomial of the algebraic variety associated with the Jukes-Cantor binary model on a trivalent tree T depends only on the number of leaves of T [BW07]. In this chapter, we ask if this property of the Hilbert polynomial can be generalized to more complex group-based models. The content in this chapter was published as [Kub12].

The most natural generalization would be the Kimura 3-parameter model, which is a group-based model with the underlying group $\mathbb{Z}_2 \times \mathbb{Z}_2$. However, we show that the Hilbert polynomial of the algebraic variety associated to the Kimura 3-parameter model depends on the shape of a trivalent tree. We do this by considering two different trees with six leaves – the caterpillar tree with six leaves and the snowflake tree, see Figure 3.1. This is the smallest interesting case with more than one trivalent tree with the same number of leaves.

The Kimura 3-parameter model being the closest model to the Jukes-Cantor binary model, it is unlikely that the property about Hilbert polynomials would hold for other models. This hypothesis was further confirmed by Donten-Bury and Michałek in [DM12]. They showed that the Hilbert polynomials of the algebraic varieties associated with the group-based models with the groups $\mathbb{Z}_3, \mathbb{Z}_4, \mathbb{Z}_5, \mathbb{Z}_7$ and a trivalent tree depend on the shape of the tree.

In Section 3.2, we recall the construction of the Kimura 3-parameter model. In Section 3.3, we show that the Hilbert polynomials of the algebraic varieties associated to the Kimura 3-parameter model on the caterpillar tree with six leaves and the snowflake tree have different values when evaluated at three, and hence their Hilbert polynomials are different. The main idea is to decompose the original trees to smaller trees and use the toric fiber product introduced by Sullivant in [Sul07]. Finally, we reduce the problem of evaluating the Hilbert polynomials of toric varieties to evaluating the Ehrhart polynomials of the corresponding polytopes. Computations are done with `polymake` [JG, JMP09] and `Normaliz` [BI].

3.2 Kimura 3-Parameter Model

First, we recall the definitions of the toric ideals and the corresponding lattice polytopes of the Kimura 3-parameter model as in Section 1.4 and [Sul07, Section 3.4]. Then we explain the toric fiber product structure on these ideals following Section 1.5 and [Sul07, Sections 1 and 3.4].

Let T be a tree with $n+1$ leaves labeled by $1,\dots,n+1$, let the root be at the leaf $n+1$, and direct the edges away from the root. A leaf l is a descendant of an edge e if there is a directed path from e to l. Denote by $\mathrm{de}(e)$ the set of all descendants of the edge e.

For a sequence $g_1,\dots,g_n$ in $\mathbb{Z}_2\times\mathbb{Z}_2$, we define

$$g_e = \sum_{i\in\mathrm{de}(e)} g_i$$

where e is an edge of T. Let

$$\mathbb{C}[q]=\mathbb{C}[q_{g_1,\dots,g_n} : g_i\in\mathbb{Z}_2\times\mathbb{Z}_2] \text{ and } \mathbb{C}[t]=\mathbb{C}[t_h^{(e)} : e\in E, h\in\mathbb{Z}_2\times\mathbb{Z}_2],$$

and consider the ring homomorphism

$$\begin{aligned}\phi_T : \mathbb{C}[q] &\to \mathbb{C}[t]\\ q_{g_1,\dots,g_n} &\mapsto \prod_{e\in E} t_{g_e}^{(e)}.\end{aligned}$$

The ideal of the Kimura 3-parameter model on a tree T is $I_T=\ker(\phi_T)$. The corresponding lattice polytope is

$$\begin{aligned}P_T=\{x\in\{0,1\}^{E\times(\mathbb{Z}_2\times\mathbb{Z}_2)} : \exists g_1,\dots,g_n\in G \text{ such that, } \forall e\in E \text{ and } \forall h\in\mathbb{Z}_2\times\mathbb{Z}_2,\\ x_h^{(e)}=1 \text{ if } h=\sum_{i\in\mathrm{de}(e)} g_i \text{ and } x_h^{(e)}=0 \text{ otherwise}\}.\end{aligned}$$

We consider P_T with respect to the lattice $L_T\subseteq\mathbb{Z}^{E\times(\mathbb{Z}_2\times\mathbb{Z}_2)}$ generated by the vertices of P_T.

Remark. There is a slight change in the notation in this chapter. Since there is no ambiguity about the group, we omit $\mathbb{Z}_2\times\mathbb{Z}_2$. We write ϕ_T, I_T, P_T, L_T instead of $\phi_{\mathbb{Z}_2\times\mathbb{Z}_2,T}, I_{\mathbb{Z}_2\times\mathbb{Z}_2,T}$, $P_{\mathbb{Z}_2\times\mathbb{Z}_2,T}, L_{\mathbb{Z}_2\times\mathbb{Z}_2,T}$, respectively.

Since T is an acyclic directed graph, there is an induced partial order on the edges of T. Namely $e<e'$ if there is a directed path from e' to e. Let e be an inner edge of T. Then e induces a decomposition of T as $T_e^+ * T_e^-$ where T_e^- is a subtree of T consisting of

all edges $e' \in T$ with $e' \leq e$ and T_e^+ consists of all edges $e' \in T$ with $e' \not\leq e$. Thus T_e^+ and T_e^- overlap in the single edge e. We root T_e^- by the tail of e, and keep the root of T_e^+ at the original root $n+1$. Without loss of generality, we may assume that the non-root leaves of T_e^+ are $\{1, 2, \ldots, m\}$ and of T_e^- are $\{e, m+1, \ldots, n\}$.

Denote by I_{T+}^e and I_{T-}^e the ideals of the Kimura 3-parameter model on the trees T_e^+ and T_e^-, and by $\mathbb{C}[q]_+$ and $\mathbb{C}[q]_-$ the ambient polynomial rings, respectively. For each variable $q_{\mathbf{g}}$ in $\mathbb{C}[q], \mathbb{C}[q]_+$, and $\mathbb{C}[q]_-$, let $\deg(q_{\mathbf{g}}) = e_{g_e}$. Let

$$\phi_{I_{T+}^e, I_{T-}^e} : \mathbb{C}[q] \to \mathbb{C}[q]_+/I_{T+}^e \otimes_{\mathbb{C}} \mathbb{C}[q]_-/I_{T-}^e$$

be the ring homomorphism such that

$$q_{g_1,\ldots,g_n} \mapsto q_{g_1,\ldots,g_m} \otimes q_{g_e,g_{m+1},\ldots,g_n}.$$

We have

$$\deg(q_{g_1,\ldots,g_n}) = \deg(q_{g_1,\ldots,g_m}) = \deg(q_{g_e,g_{m+1},\ldots,g_n}) = e_{g_e} \in \{e_{(0,0)}, e_{(0,1)}, e_{(1,0)}, e_{(1,1)}\} =: \mathcal{A}.$$

We recall that the toric fiber product of I_{T+}^e and I_{T-}^e is the kernel of $\phi_{I_{T+}^e, I_{T-}^e}$

$$I_{T+}^e \times_{\mathcal{A}} I_{T-}^e = \ker(\phi_{I_{T+}^e, I_{T-}^e}).$$

By Theorem 1.35, we have

$$I_T = I_{T+}^e \times_{\mathcal{A}} I_{T-}^e.$$

This equality will be the basis of our computations in the next section.

3.3 Counting Lattice Points

Proposition 3.1. *The Hilbert polynomials of the ideals of the Kimura 3-parameter model on the caterpillar tree with 6 leaves and the snowflake tree are different.*

Proof. Let T be a trivalent tree. In [Mic11], Michałek shows that the lattice polytope P_T is normal, hence by Theorem 1.19, its Ehrhart polynomial equals the Hilbert polynomial and the Hilbert function of I_T. This allows us to use these notions interchangeably.

1. Since the polytopes of the caterpillar with six leaves and snowflake trees are too large to compute their lattice points directly, we decompose them into smaller trees like shown in Figure 3.1.

   Henceforth, we use the abbreviations c6, sn, 3l, and 4l for the caterpillar with six leaves, snowflake, 3-leaf, and trivalent 4-leaf trees, respectively.

   For the decomposition of the caterpillar tree with 6 leaves, we define $\deg(q_{\mathbf{g}}) = e_{g_e}$ for $q_{\mathbf{g}}$ in $\mathcal{K}[q]_{\mathrm{c6}}$ and $\mathcal{K}[q]_{4\mathrm{l}}$. Then

$$I_{\mathrm{c6}} = I_{4\mathrm{l}}^e \times_{\mathcal{A}} I_{4\mathrm{l}}^e$$

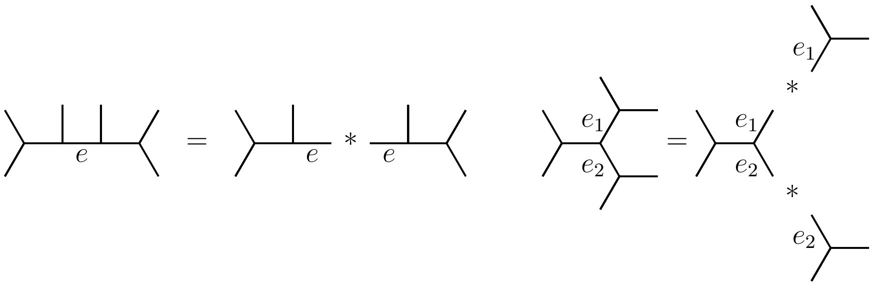


Figure 3.1: Decompositions of the caterpillar tree with six leaves and the snowflake tree

with $\mathcal{A} = \{e_{(0,0)}, e_{(0,1)}, e_{(1,0)}, e_{(1,1)}\}$.

For the decomposition of the snowflake tree, we define $\deg(q_{\mathbf{g}}) = e_{g_{e_1}, g_{e_2}}$ for $q_{\mathbf{g}}$ in $\mathcal{K}[q]_{\mathrm{sn}}$ and $\mathcal{K}[q]_{4\mathrm{l}}$, and $\deg(q_{\mathbf{g}}) = e_{g_{e_i}}$ with $i \in \{1,2\}$ for $q_{\mathbf{g}}$ in $\mathcal{K}[q]_{3\mathrm{l}}$. Then

$$I_{\mathrm{sn}} = (I_{4\mathrm{l}}^{e_1,e_2} \times_{\mathcal{A}} I_{3\mathrm{l}}^{e_1}) \times_{\mathcal{A}} I_{3\mathrm{l}}^{e_2}$$

with $\mathcal{A} = \{e_{(0,0)}, e_{(0,1)}, e_{(1,0)}, e_{(1,1)}\}$. Abusing the notation slightly, the first toric fiber product corresponds to the decomposition of the 5-leaf tree into a 4-leaf tree and a 3-leaf tree with respect to the edge e_1 and the second toric fiber product corresponds to the decomposition of the snowflake tree into the 5-leaf tree of the first fiber product and a 3-leaf tree with respect to the edge e_2.

2. Denote the multigraded Hilbert function of $\mathbb{C}[q]/I$ by $\mathrm{h}_{\mathbb{C}[q]/I}(u)$ where $u \in \mathbb{N}^{\mathbb{Z}_2\times\mathbb{Z}_2}$. By [Sul07, Corollary 2.12] the multigraded Hilbert functions of toric fiber products behave multiplicatively. Specifically, in the case of decompositions of Step 1, we get for $u, v \in \mathbb{N}^{\mathbb{Z}_2\times\mathbb{Z}_2}$

$$\mathrm{h}_{\mathbb{C}[q]_{\mathrm{c6}}/I_{\mathrm{c6}}}(u) = \mathrm{h}_{\mathbb{C}[q]_{4\mathrm{l}}/I_{4\mathrm{l}}^{e}}(u)\mathrm{h}_{\mathbb{C}[q]_{4\mathrm{l}}/I_{4\mathrm{l}}^{e}}(u),$$
$$\mathrm{h}_{\mathbb{C}[q]_{\mathrm{sn}}/I_{\mathrm{sn}}}(u,v) = (\mathrm{h}_{\mathbb{C}[q]_{4\mathrm{l}}/I_{4\mathrm{l}}^{e_1,e_2}}(u,v)\mathrm{h}_{\mathbb{C}[q]_{3\mathrm{l}}/I_{3\mathrm{l}}^{e_1}}(u))\mathrm{h}_{\mathbb{C}[q]_{3\mathrm{l}}/I_{3\mathrm{l}}^{e_2}}(v).$$

For the snowflake tree, we apply the formula twice and take into account that the edge e_2 of the 5-leaf tree belongs to the 4-leaf tree when decomposing the 5-leaf tree.

3. A monomial having multidegree $u \in \mathbb{N}^{\mathbb{Z}_2\times\mathbb{Z}_2}$ has total degree $\sum_{h\in\mathbb{Z}_2\times\mathbb{Z}_2} u_h$. Thus single graded Hilbert functions can be computed using multigraded Hilbert functions:

$$\mathrm{h}_{\mathbb{C}[q]_{\mathrm{c6}}/I_{\mathrm{c6}}}(k) = \sum_{u:\sum u_h = k} \mathrm{h}_{\mathbb{C}[q]_{\mathrm{c6}}/I_{\mathrm{c6}}}(u),$$
$$\mathrm{h}_{\mathbb{C}[q]_{\mathrm{sn}}/I_{\mathrm{sn}}}(k) = \sum_{u,v:\sum u_h = k, \sum v_h = k} \mathrm{h}_{\mathbb{C}[q]_{\mathrm{sn}}/I_{\mathrm{sn}}}(u,v).$$

4. The multigraded Hilbert function $\mathrm{h}_{\mathbb{C}[q]/I_T}(u)$ counts the lattice points in the lattice L_T of the $\sum_{h\in\mathbb{Z}_2\times\mathbb{Z}_2} u_h$ dilation of the polytope P_T intersected with the hyperplanes

$\{x_h^e = u_h\}, h \in \mathbb{Z}_2 \times \mathbb{Z}_2$. Using Step 2 and Step 3, we get for $k \in \mathbb{N}$

$$\mathrm{ehr}_{P_{c6}}(k) = \sum_{u:\sum u_h = k} \left| kP_{41} \bigcap \{x_h^e = u_h\} \bigcap L_{41} \right| \left| kP_{41} \bigcap \{x_h^e = u_h\} \bigcap L_{41} \right|,$$

$$\mathrm{ehr}_{P_{sn}}(k) = \sum_{u,v:\sum u_h = k, \sum v_h = k} \left| kP_{41} \bigcap \{x_h^{e_1} = u_h\} \bigcap \{x_h^{e_2} = v_h\} \bigcap L_{41} \right|$$
$$\cdot \left| kP_{31} \bigcap \{x_h^{e_1} = u_h\} \bigcap L_{31} \right| \left| kP_{31} \bigcap \{x_h^{e_2} = v_h\} \bigcap L_{31} \right|.$$

5. Using `polymake` and `Normaliz`, we can compute $|3P_T \cap \{x_l^e = u_l\} \cap L_T|$ for the 3-leaf and 4-leaf trees. It is important to do the basis transformation before counting the lattice points, since these programs assume that the lattice is the standard lattice. Using formulas from Step 4 we get that in the 3rd dilation the polytope of the Kimura 3-parameter model on the caterpillar tree with 6 leaves has 69324800 and the polytope of the Kimura 3-parameter model on the snowflake tree has 69248000 lattice points. Hence, their Ehrhart and Hilbert polynomials are different.

□

Remark. Similar computations show that in the 2nd dilation the polytopes of the Kimura 3-parameter model on the caterpillar tree with 6 leaves and on the snowflake tree have both 396928 lattice points.

Proposition 3.1 does not directly imply that for $n+1 \geq 7$ there exist trivalent trees T' and T'' with $n+1$ leaves such that the Hilbert polynomials of the ideals of the Kimura 3-parameter model on T' and T'' are different. However, from Proposition 3.1 follows that the multigraded Hilbert function of $\mathbb{C}[q]_{41}/I_{41}$, where the multigrading is induced by the leaves of the 4-leaf tree, depends on the labeling of the leaves. For the Jukes-Cantor binary model, this multigraded Hilbert function is independent of the labeling of the leaves [SX10, Corollary 7.12], which explains the invariance of the Hilbert polynomial.

Chapter 4

Degrees of Minimal Generators of Phylogenetic Semigroups

4.1 Introduction

Results in this chapter are a part of joint work with Weronika Buczyńska, Jarek Buczyński, and Mateusz Michałek [BBKM11]. An upper bound for the caterpillar graphs and examples for the lower bound were worked out independently by the author of this dissertation. Exposition was improved and the definition of the phylogenetic semigroup on an arbitrary graph were worked out together with the other authors of [BBKM11]. The results of [BBKM11] about the upper bound for trivalent graphs that were worked out by the other authors of [BBKM11] appeared in the dissertation of Mateusz Michałek [Mic12] and are not included here.

Let G be a graph. We study a subset $\tau(G)$ of the set of all labelings of the edges of G by integers. The set $\tau(G)$ has a natural structure of a graded semigroup with edge-wise addition. We call it the phylogenetic semigroup on G, since the conditions on the labels come from phylogenetics. The precise definition can be found in Section 4.2.

The phylogenetic semigroup on a trivalent graph was defined by Buczyńska [Buc12] as a generalization of the affine semigroup of the Jukes-Cantor binary model on a trivalent tree. In [BBKM11], we further generalized the definition of the phylogenetic semigroup to arbitrary graphs. This definition agrees with the Buczyńska's definition for trivalent graphs.

Besides phylogenetic algebraic geometry, phylogenetic semigroups appear in several other contexts. In [JW92], Jeffrey and Weitsman quantized the moduli space of flat SU(2) connections on a two-dimensional surface of genus g using a real polarization. The dimension of the quantization is counted by integral fibers of the polarization, which are in one-to-one correspondence with the labelings of a trivalent graph G with first Betti number g that satisfy the quantum Clebsch-Gordan conditions. These labelings are exactly the elements of the phylogenetic semigroup on G. Moreover, the number of the labelings that satisfy the quantum Clebsch-Gordan conditions matches the Verlinde formula for the SU(2)

Wess-Zumino-Witten model in the quantum field theory [Ver88].

In more recent work, Sturmfels and Xu showed that the projective coordinate ring of the Jukes-Cantor binary model is a sagbi degeneration of the Cox ring of the blow-up of $\mathbb{P}^{n+3}$ at n general points [SX10]. Manon generalized their construction showing that the algebra of $\mathrm{SL}_2(\mathbb{C})$ conformal blocks for a stable curve of genus g with n marked points flatly degenerates to the semigroup algebra of the phylogenetic semigroup on a graph with first Betti number g with n leaves [Man09]. The genus zero case in Manon's construction is the setting of Sturmfels and Xu.

Let G be any graph with first Betti number g. In [BBKM11], we studied the maximal degree of the minimal generating set of $\tau(G)$. It was previously known that, for $g = 0$, the phylogenetic semigroup $\tau(G)$ is generated in degree one [BW07, DM12]. For $g = 1$, Buczyńska showed that any minimal generator of $\tau(G)$ has degree at most two [Buc12]. The first main result of [BBKM11] gives an upper bound for the maximal degree of the minimal generating set of any phylogenetic semigroup.

Theorem 4.1. *Let G be a graph with first Betti number g. Any minimal generator of $\tau(G)$ has degree at most $g+1$.*

This result is not presented in this dissertation. For trivalent graphs, it appeared in the dissertation [Mic12].

We show that, for any $g \in \mathbb{N}$, there exists a graph G with first Betti number g such that the maximal degree of the minimal generating set of its phylogenetic semigroup is equal to $2\lfloor \frac{g}{2} \rfloor + 1$, i.e it is $g+1$ for g even and g for g odd. Specifically, G can be taken as the g-caterpillar graph. This implies that $g+1$ is the sharp upper bound for g even. This is the second main result of [BBKM11].

It is left open if the sharp upper bound for $g \geq 5$ odd is g or $g+1$. For $g \in \{1, 3\}$, the phylogenetic semigroup on the g-caterpillar graph has a minimal generator of degree $g+1$. For odd $g \geq 5$, we only know that the phylogenetic semigroup on the g-caterpillar graph does not have any minimal generators of degree $g+1$, unlike to the even case.

In Section 4.2, we define the phylogenetic semigroup on a graph G. In Section 4.3, we construct a degree $2\lfloor \frac{g}{2} \rfloor + 1$ indecomposable labeling of a graph with first Betti number g, and in the last section of this chapter we study labelings of the g-caterpillar graph for g odd.

4.2 Phylogenetic Semigroups

In this section, we define the phylogenetic semigroup $\tau(G)$ on a graph G. We start by recalling the definition of the lattice polytope P_T associated with the Jukes-Cantor binary model on a tree T. The phylogenetic semigroup $\tau(T)$ on a tree T is the cone over $P_T \times \{1\}$ intersected with a lattice. The phylogenetic semigroup $\tau(G)$ on a graph G is defined using the definition for trees. At the end of this section, we study some properties of the phylogenetic semigroups on trivalent trees.

We recall that the lattice polytope associated with the Jukes-Cantor binary model on a tree T is

$$P_T = \mathrm{conv}\{x \in L_T : x_e \in \{0,1\} \text{ for every } e \in E\}$$

with respect to the lattice

$$L_T = \{x \in \mathbb{Z}^E : \sum_{v \in e} x_e \in 2\mathbb{Z} \text{ for every } v \in I\}.$$

Define the associated graded lattice by

$$L_T^{gr} = L_T \oplus \mathbb{Z}$$

together with the degree map

$$\deg : L_T^{gr} = L_T \oplus \mathbb{Z} \to \mathbb{Z}$$

given by the projection on the last summand.

Definition 4.2. The phylogenetic semigroup $\tau(T)$ on T is

$$\tau(T) = \mathrm{cone}(P_T \times \{1\}) \cap L_T^{gr}.$$

Definition 4.3. The *First Betti number* of a graph is the minimal number of cuts that would make the graph into a tree.

Remark. Given the connection between phylogenetic semigroups and conformal block algebras, it is tempting to say *genus* of a graph instead of the first Betti number. However, this is inconsistent with the graph theory notation, where genus of a graph is the smallest genus of a surface such that the graph can be embedded into that surface.

To a given graph G with first Betti number g we associate a tree T with g distinguished pairs of leaf edges with the aim of defining $\tau(G)$ based on $\tau(T)$. This procedure can be described inductively on g. If $g = 0$, then the graph is a tree with no distinguished pairs of leaf edges. For $g > 0$, we choose a cycle edge e. We divide e into two edges $\underline{e}$ and $\overline{e}$, adding two vertices $\underline{l}$ and $\overline{l}$ of valency 1. The edges $\underline{e}$ and $\overline{e}$ form a distinguished pair of leaf edges. This procedure decreases the first Betti number by one and increases the number of distinguished pairs by one. Usually the resulting tree with distinguished pairs of leaf edges is not unique. However, a tree with distinguished pairs of leaf edges encodes precisely one graph and the following definition does not depend on the resulting tree.

Definition 4.4. Let G be a graph. Let T be an associated tree with a set of distinguished pairs of leaves $\{(\underline{e_i}, \overline{e_i})\}$. We define the *phylogenetic semigroup on G* as

$$\tau(G) = \tau(T) \cap \bigcap_i (x_{\underline{e_i}} = x_{\overline{e_i}}).$$

In other words, $\tau(G)$ consists of those labelings of $\tau(T)$ where the label on $\underline{e_i}$ is identical to the one on $\overline{e_i}$, and thus the labeling of T gives a labeling of G. Similarly, define the lattice

$$L_G^{gr} = L_T^{gr} \cap \bigcap_i (x_{\underline{e_i}} = x_{\overline{e_i}})$$

together with the degree map induced by the degree map of L_T^{gr}.

Remark. If we knew inequality descriptions of the phylogenetic semigroups on all claw trees, then it would be easy to define the phylogenetic semigroup on any graph using these inequality descriptions. Unfortunately, inequality descriptions of phylogenetic semigroups are not known for general claw trees, and we have to use a point description to define the phylogenetic semigroup on a graph. An inequality description of the phylogenetic semigroup on a trivalent graph is given in Lemma 4.6.

By Gordan's Lemma, the phylogenetic semigroup $\tau(G)$ has a unique minimal generating set. We call the elements of the minimal generating set minimal generators, or sometimes also indecomposable elements of $\tau(G)$.

Finally, we study some properties of the phylogenetic semigroups on trivalent graphs that we will need in the next sections.

Notation. Let G be a trivalent graph and v be an inner vertex of G. Let $\{e_1, e_2, e_3\}$ be the edges of ⅄ and i_v : ⅄ $\hookrightarrow G$ be a map that is locally an embedding and sends the central vertex of ⅄ to v. For $\omega \in L_G^{gr}$, we denote

$$a_v(\omega) := \omega_{i_v(e_1)}, \quad b_v(\omega) := \omega_{i_v(e_2)}, \quad c_v(\omega) := \omega_{i_v(e_3)}.$$

In other words, a_v, b_v, c_v measure the coefficients of ω at the edges incident to v.

Definition 4.5. The *degree* of $\omega \in L_G^{gr}$ *at an inner vertex* $v \in I$ is

$$\deg_v(\omega) := \frac{1}{2}\big(a_v(\omega) + b_v(\omega) + c_v(\omega)\big).$$

Lemma 4.6 ([Buc12], Definition 2.18 and Lemma 2.23)**.** *For a trivalent graph G, the phylogenetic semigroup $\tau(G)$ on G is the set of elements ω satisfying the following conditions*

[$\heartsuit$]. *parity condition:* $\omega \in L_G^{gr}$*,*

[+]. *non-negativity condition:* $\omega_e \geq 0$ *for any* $e \in E$*,*

[$\triangle$]. *triangle inequalities:* $|a_v(\omega) - b_v(\omega)| \leq c_v(\omega) \leq a_v(\omega) + b_v(\omega)$ *for each inner vertex* $v \in I$*,*

[$^\circ$]. *degree inequalities:* $\deg(\omega) \geq \deg_v(\omega)$ *for any* $v \in I$*.*

The triangle inequalities [$\triangle$] are symmetric and do not depend on the embedding i_v.

Remark. If every connected component of G contains at least one inner vertex, then the inequalities above imply $\deg(\omega) \geq \omega_e$ for all edges. However, if G contains connected components that contain only a single edge e, then the inequality $\deg(\omega) \geq \omega_e$ should be included in Lemma 4.6.

Finally, we prove that trivalent graphs have the highest degree minimal generating sets among all graphs with the same first Betti number. This knowledge is helpful for the search of graphs with high degree indecomposable elements as we can limit ourselves to trivalent graphs.

Lemma 4.7. *Let G be a graph with first Betti number g. Assume that the maximal degree of the minimal generating set of $\tau(G)$ is n. Then there exists a trivalent graph G' with first Betti number g such that the maximal degree of the minimal generating set of $\tau(G')$ is at least n.*

Proof. We construct G' from G. Choose an inner vertex v of G that is not trivalent. Replace v by v' and v'' together with a new edge between them, let two edges incident to v be incident to v' and the rest of the edges incident to v be incident to v''. After a finite number of replacements we get a trivalent graph G', because $valency(v') < valency(v)$ and $valency(v'') < valency(v)$.

Now consider a tree T with g distinguished pairs of leaf edges associated to G that is attained by dividing edges $e_1, e_2, \dots, e_g$ into two. Dividing exactly the same edges $e_1, e_2, \dots, e_g$ into two in G' gives a tree T' with g distinguished pairs of leaf edges associated to G'. As $\tau(T)$ and $\tau(T')$ are normal [DM12, Proposition 3.12], the semigroup $\tau(T)$ is a coordinate projection of the semigroup $\tau(T')$ that forgets coordinates corresponding to new edges. Hence, the semigroup $\tau(G)$ is a coordinate projection of the semigroup $\tau(G')$ and the projections of the minimal generators of $\tau(G')$ generate $\tau(G)$. □

4.3 Sharpness of the Upper Bound for Even g

In this section, we show that if g is even then the bound $g+1$ is sharp for the caterpillar graph with g loops.

Definition 4.8. The trivalent graph obtained from the caterpillar tree with $g+1$ leaves by attaching a loop to all but one leaf (the leftmost one) as illustrated in Figure 4.1 is called the *g-caterpillar graph.*

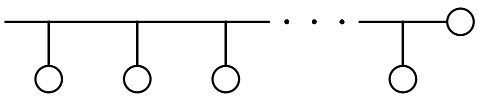


Figure 4.1: The g-caterpillar graph

Lemma 4.9. *Let G be the g-caterpillar graph and $\omega \in L_G^{gr}$. Then ω_e is even on every edge e other than loops.*

Proof. The statement follows directly from the parity condition for the edges incident to loops, and thus for all edges. □

The tripod contains three non-empty paths, each consisting of two edges. Denote them by

$$x := e_2 + e_3, \quad y := e_1 + e_3, \quad z := e_1 + e_2$$

where $\{e_1, e_2, e_3\}$ are edges of the tripod. Together with the empty path, they correspond to the minimal generators of the phylogenetic semigroup $\tau(\text{人})$. Since $\tau(\text{人})$ is normal, every element of the semigroup can be written as a sum of paths x, y, z, and the empty path. Moreover, since the minimal generators of $\tau(\perp)$ are vertices of a simplex, this decomposition is unique.

Now let G be any trivalent graph. Similarly to the tripod case, at every inner vertex v of G, we can write an element of $\tau(G)$ as a unique sum of paths x, y, z, and the empty path. In the case of the g-caterpillar graph, we denote the local paths at an inner vertex v on the horizontal line *straight*, *left*, and *right* paths, as shown in Figure 4.2.

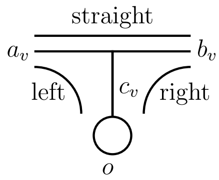


Figure 4.2: Notation for local paths at a vertex of the g-caterpillar graph

Corollary 4.10. *Let G be a g-caterpillar graph, $\omega \in \tau(G)$, and v a vertex not on a loop. Then*

- *if* $\deg_v \omega$ *is even, then the number of straight (left, right) paths at v is even,*
- *if* $\deg_v \omega$ *is odd, then the number of straight (left, right) paths at v is odd.*

In particular, $\deg_v(\omega) \neq 1$.

Now we are ready to prove that for g even the g-caterpillar graph has degree $g+1$ indecomposable elements.

Example 4.11. Suppose $g = 2k$, and let G be the g-caterpillar graph. The element ω defined in Figure 4.3 is indecomposable.

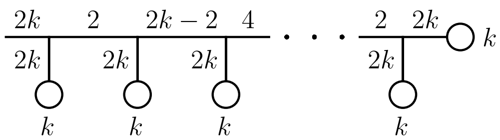
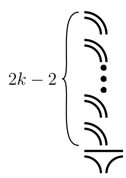
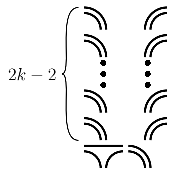


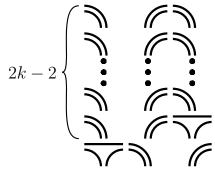
Figure 4.3: The indecomposable element ω of degree $g+1$

Proof. We begin the proof by explaining the local decomposition of ω. Starting from the left-most inner vertex of the caterpillar tree we have

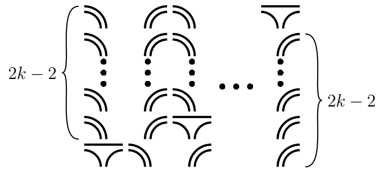
(1) $2k-1$ left, 1 right, 1 straight paths



(2) $2k-2$ right, 2 left paths 

(3) $2k-3$ left, 3 right, 1 straight paths 

$\vdots \quad \vdots$

$(2k-1)$ 1 left, $2k-1$ right, 1 straight paths 

Suppose for a contradiction that ω is decomposable as $\omega' + \omega''$. Since the degree of ω is odd, one of the two parts has even degree. Assume ω' has even degree $\deg(\omega') = 2i$ with $i > 0$.

Every second vertex v on the horizontal line has a single straight line in the local decomposition of ω. Moreover at such v the degree is attained $\deg_v \omega = \deg \omega$. Thus $\deg_v \omega' = \deg \omega'$ and $\deg_v \omega'' = \deg \omega''$ as well. By Corollary 4.10, the local decomposition of ω'' at v consists of the single straight path and odd number of left paths and odd number of right paths, whereas the local decomposition of ω' at v consists of even number of left paths and even number of right paths. This means ω' must have $2i$ left paths at the left-most inner vertex on the horizontal line of G. At the next inner vertex on the horizontal line, ω' has $2i$ right paths by Example 4.9, and so on. This is a contradiction, as at some inner vertex on the horizontal line ω has less than $2i$ left paths. $\square$

4.4 A Lower Bound for Odd g

Example 4.12. Suppose $g = 2k+1$, and let G be the g-caterpillar graph. By extending the labeling from Example 4.11 to the extra loop of the $(g+1)$-caterpillar, we get a degree g indecomposable labeling of G.

Hence, for g odd, there exists a graph with first Betti number g such that its phylogenetic semigroup has a minimal generator of degree g. We will show that, for g odd, the maximal degree of the minimal generating set of the phylogenetic semigroup on the g-caterpillar graph is g, unlike to the even case. The question whether, for g odd, there exists a graph with first Betti number g and this maximal degree equal to $g+1$ is left open.

Lemma 4.13. *Let G be the g-caterpillar graph. Let $\omega \in \tau(G)$ be an element of even degree at least 6. Then ω can be decomposed into degree 2 and $\deg(\omega) - 2$ elements.*[1]

Proof. For this proof, we fix the following notation. At each vertex v on the horizontal line of the g-caterpillar, we choose an embedding of the tripod so that a_v, b_v, and c_v are arranged as in Figure 4.2, so c_v is the value on the vertical edge, a_v on the left one, b_v on the right one.

Let $d := \deg(\omega)$ be the degree of ω. We will define a degree 2 element ω', so that $\omega = \omega' + \omega''$ is a decomposition in $\tau(G)$. In our construction we use local paths. This assures that the resulting ω' and ω'' fulfill the triangle inequalities [$\triangle$] of $\tau(G)$. To assure the degree inequalities [$^\circ$], we require that ω' satisfies the following at each inner vertex v

$$d - 2 \geq \deg_v(\omega'') = \deg_v(\omega) - \deg_v(\omega'). \tag{4.1}$$

Note that if $\deg_v(\omega') = 2$, or equivalently, if ω' is constructed using two local paths at v, then (4.1) is automatically fulfilled.

First, we define the labels of ω' on the caterpillar tree, ignoring the labels on the loops for a while. We define them inductively from left to right using local paths, in such a way that the following condition holds for every inner vertex v of the caterpillar tree

$$b_v(\omega') = \begin{cases} 0 & \text{if } b_v(\omega) < \frac{d}{2}, \\ 2 & \text{if } b_v(\omega) > \frac{d}{2}, \\ 0 \text{ or } 2 & \text{otherwise.} \end{cases} \tag{4.2}$$

First, we define ω' for the left-most edge e

$$\omega'_e = \begin{cases} 0 & \text{if } \omega_e \leq \frac{d}{2}, \\ 2 & \text{otherwise.} \end{cases}$$

We need to prove that at every step there is enough of local paths in ω to fulfill conditions (4.1) and (4.2). There are six cases depending on the value of ω' on the previous edge and the value of ω on the current one.

1. If $a_v(\omega') = 2$ and $b_v(\omega) > d/2$, then we have to prove that ω has at least two straight paths at v, since we need $b_v(\omega') = 2$. The condition (4.2) gives $a_v(\omega) \geq d/2$, and

   $$\#\text{straight} = \frac{a_v(\omega) + b_v(\omega) - c_v(\omega)}{2} > \frac{d}{2} - \frac{c_v(\omega)}{2} > 0,$$

   where the last inequality holds because of

   $$2d \geq a_v(\omega) + b_v(\omega) + c_v(\omega) > \frac{d}{2} + \frac{d}{2} + c_v(\omega) = d + c_v(\omega).$$

   As d and $c_v(\omega)$ are both even, we conclude that ω has at least two straight paths at v.

[1] The improved version of the proof that we present here is in large extent due to Weronika Buczyńska and Jarek Buczyński.

2. If $a_v(\omega') = 2$ and $b_v(\omega) = d/2$, then we have to prove that ω has either at least two straight paths or at least two left paths at v, since we need either $b_v(\omega') = 2$ or $b_v(\omega') = 0$. The condition (4.2) gives $a_v(\omega) \geq d/2$, and

$$\#\text{straight} + \#\text{left} = a_v(\omega) \geq \frac{d}{2} \geq 3.$$

3. If $a_v(\omega') = 2$ and $b_v(\omega) < d/2$, then we have to prove that ω has at least two left paths at v, since we need $b_v(\omega') = 0$. The condition (4.2) gives $a_v(\omega) \geq d/2$, and thus $a_v(\omega) - b_v(\omega) > 0$. By the triangle inequalities [△], we have

$$\begin{aligned}\#\text{left} = \frac{c_v(\omega) + a_v(\omega) - b_v(\omega)}{2} &\geq \frac{a_v(\omega) - b_v(\omega)}{2} + \frac{|a_v(\omega) - b_v(\omega)|}{2} \\ = a_v(\omega) - b_v(\omega) \geq 1\end{aligned}$$

   As $a_v(\omega)$ and $b_v(\omega)$ are both even, we conclude that ω has at least two left paths at v.

4. If $a_v(\omega') = 0$ and $b_v(\omega) > d/2$, then we have to prove that ω has at least two right paths at v, since we need $b_v(\omega') = 2$. The condition (4.2) gives $a_v(\omega) \leq d/2$, and thus $b_v(\omega) - a_v(\omega) > 0$. Again, by the triangle inequalities [△] we have

$$\begin{aligned}\#\text{right} = \frac{c_v(\omega) + b_v(\omega) - a_v(\omega)}{2} &\geq \frac{b_v(\omega) - a_v(\omega)}{2} + \frac{|b_v(\omega) - a_v(\omega)|}{2} \\ = b_v(\omega) - a_v(\omega) \geq 1\end{aligned}$$

5. If $a_v(\omega') = 0$ and $b_v(\omega) = d/2$, we have to prove that either $\deg_v(\omega) \leq d - 2$ or ω has two right paths at v, since we need either $b_v(\omega') = 0$ or $b_v(\omega') = 2$. If $\deg_v(\omega) \geq d - 1$, using the condition (4.2) gives

$$\#\text{right} = \frac{b_v(\omega) + c_v(\omega) - a_v(\omega)}{2} = \deg_v(\omega) - a_v(\omega) \geq (d-1) - \frac{d}{2} \geq 2.$$

6. If $a_v(\omega') = 0$ and $b_v(\omega) < d/2$, then we have to prove that $\deg_v(\omega) \leq d - 2$, since we need $b_v(\omega') = 0$. The condition (4.2) gives $a_v(\omega) \leq d/2$, and thus $a_v(\omega) + b_v(\omega) \leq d-1$. As $a_v(\omega)$ and $b_v(\omega)$ are both even, we even have $a_v(\omega) + b_v(\omega) \leq d - 2$. Using this and the triangle inequalities [△], we get the desired inequality:

$$2\deg_v(\omega) = a_v(\omega) + b_v(\omega) + c_v(\omega) \leq d - 2 + c_v(\omega) \leq d - 2 + a_v(\omega) + b_v(\omega) \leq 2d - 4.$$

Note that we use $d \geq 6$ only in cases with $b = d/2$, i.e., cases 2 and 5.

It remains to suitably define the labels of ω' on the loops. Fix a loop o. In the local decomposition of ω at the vertex v_o some of the local paths come in pairs: There are $\omega_{e_o}/2$ loops with 2 on the adjacent edge and 1 on the loop; there are $(\omega_o - \omega_{e_o}/2)$ single loops with 0 on the adjacent edge and 1 on the loop.

If $\omega'_{e_o} = 2$ then $\omega_{e_o} \geq 2$, and there is at least one loop with 2 on the adjacent edge in the local decomposition of ω. Set $\omega'_o = 1$.

Otherwise $\omega'_{e_o} = 0$ by the construction above. This implies together with the Remark 4.2 that $\omega_{e_o} \leq d - 2$. Hence, the number of single loops

$$\omega_o - \omega_{e_o}/2 = \deg_{v_o}(\omega) - \omega_{e_o} \geq \deg_{v_o}(\omega) - d + 2,$$

and we define

$$\omega'_o = \max\{\deg_{v_o}(\omega) - d + 2, 0\}.$$

Finally, we check that the condition (4.1) is fulfilled.

$$\deg_{v_o}(\omega) - \deg_{v_o}(\omega') \leq \deg_{v_o}(\omega) - (\deg_{v_o}(\omega) - d + 2) \leq d - 2.$$

This completes the proof. $\square$

Chapter 5

Low Degree Minimal Generators of Phylogenetic Semigroups

5.1 Introduction

This chapter continues the study of phylogenetic semigroups started in the previous chapter, where we studied the maximal degrees of the minimal generators of phylogenetic semigroups. The aim of this chapter is to explicitly characterize the minimal generators of low degree of phylogenetic semigroups.

The minimal generators of low degree of phylogenetic semigroups have been previously studied for trees and graphs with first Betti number 1. The phylogenetic semigroups on trees are generated by degree one labelings, known as networks [BW07, DM12]. Buczyńska studied the minimal generators of the phylogenetic semigroups on the trivalent graphs with first Betti number 1. She proved that any minimal generator of the phylogenetic semigroup on a trivalent graph with first Betti number 1 has degree at most two, and explicitly described the minimal generating sets [Buc12].

In this chapter, we extend this result from trivalent graphs to general graphs: We describe the minimal generating set of the phylogenetic semigroup on any graph with first Betti number $g \leq 1$. Moreover, we characterize the minimal generators of degree two of the phylogenetic semigroups on all trivalent graphs with first Betti number $g > 1$.

We also specify the bound on the maximal degree of the minimal generating set for all graphs with first Betti number 2. By [BBKM11], the maximal degree of the minimal generating set of the phylogenetic semigroup on a graph with first Betti number 2 is at most three. We explicitly characterize when the maximal degree three is attained, and when the maximal degree is equal to two or one. If the degree three is attained, we describe the minimal generators of degree three.

In the last section of this chapter, we list the maximal degrees of the minimal generating sets of the phylogenetic semigroups on some graphs with first Betti number 3, 4, or 5. We speculate that the maximal degree depends on the separateness of the cycles of the graph. Having low maximal degree is especially interesting from the perspective of $\mathrm{SL}_2(\mathbb{C})$

conformal block algebras as this ensures a low maximal degree for the minimal generators of these algebras, see [Man12b].

In Section 5.2, we give a shortened proof of a Buczyńska's theorem about the minimal generators of the phylogenetic semigroups on the trivalent graphs with first Betti number 1, and we generalize the statement to general graphs with first Betti number 1. In Section 5.3, we characterize the minimal generators of degree two for any trivalent graph. In Section 5.4, we study the explicit maximal degree of the minimal generating set of the phylogenetic semigroup on a graph with first Betti number 2, and in some cases describe the minimal generating sets of the phylogenetic semigroups on graphs with first Betti number 2. In Section 5.5, we complete the description of the minimal generating sets of the phylogenetic semigroups on the trivalent graphs with first Betti number 2. In the last section, we list examples of these maximal degrees for graphs with first Betti numbers 3,4, and 5.

5.2 Graphs with First Betti Number 1

In this section, we study the minimal generating sets of the phylogenetic semigroups on the graphs with first Betti number 1. Buczyńska did this for trivalent graphs [Buc12]. We give a shortened proof of her result, and as a corollary, we describe the minimal generating set of the phylogenetic semigroup on any graph with first Betti number 1.

Definition 5.1. Let G be a graph. A *path* in G is a sequence of unrepeated edges which connect a sequence of vertices. Moreover, we require the first and the last vertex to be either both leaves or equal. In the latter case, a path is called a *cycle*. A *network* is a disjoint union of paths. A *cycle edge* is an edge on a cycle of G. A *cycle leg* is an edge incident to a cycle edge, but is not a cycle edge.

Let G be a graph and $\overline{e}$ an inner edge of G. Let e' and e'' be new leaf edges obtained by cutting G at $\overline{e}$, as illustrated in Figure 5.1. Then $\omega \in \tau(G)$ gives an element $\overline{\omega} \in \tau(G^{\overline{e}})$:

$$\overline{\omega}_e = \begin{cases} \omega_e & \text{if } e \notin \{e', e''\}, \\ \omega_{\overline{e}} & \text{if } e \in \{e', e''\}. \end{cases}$$

On the contrary, given $\overline{\omega} \in \tau(G^{\overline{e}})$, it gives an element $\omega \in \tau(G)$ if and only if $\overline{\omega}_{e'} = \overline{\omega}_{e''}$:

$$\omega_e = \begin{cases} \overline{\omega}_e & \text{if } e \neq \overline{e}, \\ \overline{\omega}_{e'} & \text{if } e = \overline{e}. \end{cases}$$

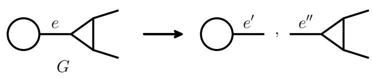


Figure 5.1: A graph $G^{\overline{e}}$ obtained by cutting an inner edge $\overline{e}$ of G

In [Buc12], a polygon graph G was defined as a graph with $2k$ edges, k of which form the only cycle of G and the remaining k edges are cycle legs. The use of polygon graphs simplifies the study of the phylogenetic semigroups on the trivalent graphs with first Betti number 1. We generalize this definition to be able to simplify the study of the phylogenetic semigroups on any graph.

Definition 5.2. A graph G with first Betti number $g \geq 1$ is called a *multiple polygon graph* if for no edge e we can write $G^e = G' \sqcup G''$ with G' or G'' a tree with more than one edge, see Figure 5.2 for examples. A multiple polygon graph is a *polygon graph* if it has first Betti number 1.

Lemma 5.3. *Given a graph G with first Betti number $g \geq 1$, there exist non-cycle inner edges $e_1, \ldots, e_k$ of G such that $G^{e_1,\ldots,e_k} = G_0 \sqcup G_1 \sqcup \ldots \sqcup G_k$ where G_0 is a multiple polygon graph and $G_1, \ldots, G_k$ are trees.*

Proof. Choose all non-cycle edges e such that we can write $G^e = G' \sqcup G''$ with G'' a tree with more than one edge and e maximal with this property, i.e. there is an edge $\overline{e}$ incident to e such that we cannot write $G^{\overline{e}} = G' \sqcup G''$ with G' or G'' a tree. $\square$

Lemma 5.4. *Let G be a graph and $\omega \in \tau(G)$. Let e be a non-cycle inner edge such that $G^e = G' \sqcup G''$ with G'' a tree. Then any decomposition of $\omega|_{G'} \in \tau(G')$ lifts to a decomposition of $\omega \in \tau(G)$.*

Proof. This lemma is stated for trivalent graphs in [Buc12, Lemma 2.31]. Since $\tau(T)$ is normal for any tree T [DM12, Proposition 18], then the proof works for the general case exactly the same way as it does for the trivalent case. $\square$

Corollary 5.5. *Let G be a graph and $\omega \in \tau(G)$. Let $e_1, \ldots, e_k$ be non-cycle inner edges such that $G^{e_1,\ldots,e_k} = G_0 \sqcup G_1 \sqcup \ldots \sqcup G_k$ where G_0 is a multiple polygon graph and $G_1, \ldots, G_k$ are trees. Then any decomposition of $\omega|_{G_0} \in \tau(G_0)$ lifts to a decomposition of $\omega \in \tau(G)$.*

Proof. We can use Lemma 5.4 iteratively. $\square$

Networks can be seen as degree one elements of $\tau(G)$. We define ω corresponding to a network Γ in the following way:

$$\omega_e = \begin{cases} 1 & \text{if } e \text{ belongs to } \Gamma, \\ 0 & \text{otherwise.} \end{cases}$$

It follows from the definition of a network that the parity condition is fulfilled for ω at every inner vertex of G. Hence $\omega \in \tau(G)$. We will often use the notion network for the corresponding labeling $\omega \in \tau(G)$.

It has been shown for various classes of graphs that networks are in one-to-one correspondence with the degree one elements of a phylogenetic semigroup [BW07, Lemma 3.3], [Buc12, Lemma 2.26]. For an arbitrary tree, this was stated in [BBKM11, Section 2], but no proof was given. We did not find proofs for arbitrary trees or graphs in the literature, and therefore will present them here.

Lemma 5.6. *Let T be a tree. There is a one-to-one correspondence between the networks and the degree one elements of $\tau(T)$.*

Proof. We will prove the lemma by induction on the number of inner vertices of T.
Base case: The statement of the lemma clearly holds for claw trees.
Induction step: Let T be a tree with $n > 1$ inner vertices and $\omega \in \tau(T)$ a degree one labeling. If T has more than one connected component, then by induction ω restricted to any connected component is a disjoint union of paths. Hence, the labeling ω is a disjoint union of paths.

If T has one connected component, let e be an inner edge, e_1, e_2 new leaf edges obtained by cutting T at e and write $T^e = T_1 \sqcup T_2$. Then ω restricted to either tree is a disjoint union of paths. If $\omega_e = 0$, then ω is the disjoint union of exactly the same paths. If $\omega_e = 1$, then the path of T_1 containing e_1 and the path of T_2 containing e_2 are combined to one path of T containing e. Hence, the labeling ω is a disjoint union of paths. □

Lemma 5.7. *Let G be a graph. There is a one-to-one correspondence between the networks and the degree one elements of $\tau(G)$.*

Proof. We will prove the lemma by induction on the first Betti number g of G.
Base case: The statement of the lemma holds for trees by Lemma 5.6.
Induction step: Let G be a graph with first Betti number $g > 1$ and $\omega \in \tau(G)$ a degree one labeling. Let e be a cycle edge of G and e_1, e_2 new leaf edges obtained by cutting G at e. The graph G^e has first Betti number $g - 1$. Then ω gives $\overline{\omega} \in G^e$ that is a disjoint union of paths containing both e_1, e_2 or neither of them. If $\omega_e = 0$, then ω is the disjoint union of exactly the same paths. If $\omega_e = 1$, then there are two possibilities. Either there is a path in $\overline{\omega}$ with the first edge e_1 and the last edge e_2 which lifts to a cycle in ω. Or there is a path in $\overline{\omega}$ with the first edge e' and the last edge e_1, and another path in $\overline{\omega}$ with the first edge e_2 and the last edge e'' where e', e'' are leaf edges. These paths in $\overline{\omega}$ lift to a single path in ω with the first edge e and the last edge e' in G. □

Corollary 5.8. *Let G be a graph. All networks are included in the minimal generating set of $\tau(G)$.*

Proof. For any graded affine semigroup $\mathbb{N}\mathcal{A}$, all minimal generators of degree one are included in the minimal generating set of $\mathbb{N}\mathcal{A}$. □

Theorem 5.9 ([Buc12], Theorem 2.29)**.** *Let G be a trivalent graph with first Betti number 1 and $\omega \in \tau(G)$. Then ω is a minimal generator of $\tau(G)$ if and only if it satisfies one of the following conditions:*

- *ω is a network, or*
- *ω has degree two, and satisfies the following three conditions:*
  - *(i)* $\omega_e = 1$ *for all cycle edges e,*
  - *(ii)* $\omega_e = 2$ *for an odd number of cycle legs,*

(iii) $\omega_e = 0$ *for the remaining cycle legs.*

We give a shortened proof of this theorem. The following lemma will be an important part of it.

Lemma 5.10. *Let G be a graph with first Betti number 1. Let $\omega \in \tau(G)$ be of degree d. If there is a cycle edge e with $\omega_e = 0$ or $\omega_e = d$, then ω decomposes as a sum of degree one elements.*

Proof. Let e be a cycle edge and e_1, e_2 new leaf edges obtained by cutting G at e. Notice that G^e is a tree. Then ω gives $\overline{\omega} \in \tau(G^e)$ that decomposes into degree one elements $\overline{\omega} = \overline{\omega_1} + \ldots + \overline{\omega_d}$. Since $(\overline{\omega_i})_{e_1} = (\overline{\omega_i})_{e_2}$ for all i, the decomposition $\overline{\omega} = \overline{\omega_1} + \ldots + \overline{\omega_d}$ gives a decomposition $\omega = \omega_1 + \ldots + \omega_d$ of $\omega \in \tau(G)$. $\square$

Proof of Theorem 5.9. By Corollary 5.5 we can assume that G is a trivalent polygon graph. First, we prove that any minimal generator of $\tau(G)$ has degree at most two. Let $\omega \in \tau(G)$ be of degree d. Let e be a cycle edge and e_1, e_2 new leaf edges obtained by cutting G at e. Then ω gives $\overline{\omega} \in \tau(G^e)$ that decomposes as a sum of degree one elements $\overline{\omega} = \overline{\omega_1} + \ldots + \overline{\omega_d}$. If $(\overline{\omega_i})_{e_1} = (\overline{\omega_i})_{e_2}$ then $\overline{\omega_i}$ gives an element $\omega_i \in \tau(G)$. Otherwise there exists j such that $(\overline{\omega_i})_{e_1} = (\overline{\omega_j})_{e_2}$ and $(\overline{\omega_j})_{e_1} = (\overline{\omega_i})_{e_2}$, because $\overline{\omega}_{e_1} = \overline{\omega}_{e_2}$. Thus $\overline{\omega_i} + \overline{\omega_j}$ gives a degree two element $\omega_i + \omega_j \in \tau(G)$.

The degree one elements of $\tau(G)$ are networks by Corollary 5.7. By Lemma 5.10, all degree two indecomposable elements ω have $\omega_e = 1$ on all cycle edges e. Since G is a trivalent graph, we have $\omega_e \in \{0, 2\}$ for all cycle legs because of the parity condition. Assume $\omega_e = 2$ for an even number of cycle legs $e_1, \ldots e_{2k}$ in clockwise order. Denote by P_i the path starting at e_i and ending at e_{i+1} (at e_0 for $i = 2k$). Then ω decomposes as the sum of networks $P_1 \cup P_3 \cup \ldots \cup P_{2k-1}$ and $P_2 \cup P_4 \cup \ldots \cup P_{2k}$. Hence, for ω indecomposable, $\omega_e = 2$ for an odd number of cycle legs.

Conversely, assume that $\omega \in \tau(G)$ has degree two and fulfills $(i), (ii), (iii)$. Suppose $\omega = \omega_1 + \omega_2$ where ω_1, ω_2 are networks. For all cycle legs e with $\omega_e = 2$, we have $(\omega_i)_e = 1$, since $(\omega_i)_e \leq 1$ for all edges e. Hence, we have $(\omega_i)_e = 1$ for odd number of leaves of G. But this is contradiction to the fact that ω_i is a network. $\square$

Remark. We know from [Buc12, BBKM11] that a minimal generator of the phylogenetic semigroup on a graph with first Betti number 1 has degree at most two. We showed this above to give a simple and self-containing proof.

Corollary 5.11. *Let G be a graph with first Betti number 1 and $\omega \in \tau(G)$. Then ω is a minimal generator of $\tau(G)$ if and only if it satisfies one of the following conditions:*

- *ω is a network, or*
- *ω has degree two, and satisfies the following three conditions:*

  (i) $\omega_e = 1$ *for all cycle edges e,*

  (ii) $\omega_e = 2$ *for an odd number of cycle legs,*

(iii) $\omega_e = 0$ *for the remaining cycle legs.*

Proof. Let G' be a trivalent graph constructed from G in the following way: Replace all vertices v with valency higher than three by two new vertices v' and v'' together with a new edge between them, let two edges incident to v be incident to v' and the rest of the edges incident to v be incident to v''. Moreover, if v is on the cycle, let one cycle edge incident to v be incident to v' and let the other cycle edge incident to v be incident to v''. This assures that we do not add any cycle legs. After a finite number of replacements we get a trivalent graph G'. By the proof of Lemma 4.7, $\tau(G)$ is the coordinate projection of $\tau(G')$ that forgets coordinates corresponding to new edges. In particular, if $\omega' \in \tau(G')$ is decomposable, then its projection in $\tau(G)$ is also decomposable.

By [BBKM11], any minimal generator of $\tau(G)$ has degree at most two. Degree one elements are networks. We are left with describing the indecomposable elements of degree two of $\tau(G)$. A degree two indecomposable element $\omega \in \tau(G)$ is the coordinate projection of a degree two indecomposable element of $\tau(G')$. Since all cycle legs of G' are also cycle legs of G, then by Theorem 5.9 the conditions $(i), (ii), (iii)$ are fulfilled for ω.

Conversely, assume that the conditions $(i), (ii), (iii)$ are fulfilled. Suppose $\omega = \omega_1 + \omega_2$ where ω_1, ω_2 are networks. For all cycle legs e with $\omega_e = 2$, we have $(\omega_i)_e = 1$, since $(\omega_i)_e \leq 1$ for all edges e. Hence, we have $(\omega_i)_e = 1$ for odd number of leaves of G'. But this is a contradiction to the fact that ω_i is a network. ☐

5.3 Minimal Generators of Degree Two

In this section, we describe degree two indecomposable labelings for any trivalent graph G.

Lemma 5.12. *Let G be any graph and $\omega \in \tau(G)$ a degree two labeling. If there exists a cycle G' of G such that $\omega_e = 1$ for all cycle edges $e \in G'$, $\omega_e = 2$ for an odd number cycle legs e of G' and $\omega_e = 0$ for the remaining cycle legs $e \in G'$, then the labeling ω is indecomposable.*

Proof. If ω decomposes, then a decomposition of ω restricts to a decomposition of $\omega|_{G'} \in \tau(G')$ where G' is a cycle together with its cycle legs. Thus the statement follows from Corollary 5.11. ☐

Lemma 5.13. *Let G be a trivalent graph and $\omega \in \tau(G)$ a degree two labeling. The labeling ω is indecomposable if and only if there exists a cycle G' of G together with its cycle legs such that $\omega|_{G'} \in \tau(G')$ is indecomposable.*

Proof. One direction follows from Lemma 5.12. We show by induction on the first Betti number of G that if $\omega \in \tau(G)$ is a degree two indecomposable labeling then there exists a cycle G' together with its cycle legs such that $\omega|_{G'}$ is a degree two indecomposable labeling.

Base case: If the first Betti number of G is 1, then the statement follows from Theorem 5.9.

Induction step: Assume that the first Betti number of G is $g > 1$. If more than one connected component of G contains a cycle, then there exists a connected component C of

G containing a cycle such that $\omega|_C \in \tau(C)$ is an indecomposable element of degree two. Since the first Betti number of C is less than g, we know by induction that there exists a cycle G' of C together with its cycle legs such that $\omega|_{G'} \in \tau(G')$ is an indecomposable element of degree two.

Otherwise all cycles of G live in the same connected component of G. If $\omega_e = 1$ for all cycle edges e, then by the parity condition $\omega_e \in \{0, 2\}$ for all cycle legs e. In particular, none of the cycle legs is simultaneously a cycle edge and there exists a cycle leg e that separates some cycles of G. Let e_1, e_2 be the new leaf edges obtained by cutting G at e and write $G^e = G_1 \sqcup G_2$. Then ω gives $\omega_1 \in \tau(G_1)$ and $\omega_2 \in \tau(G_2)$ with at least one of them indecomposable, otherwise one could lift these decompositions to a decomposition of ω. By induction, for i with ω_i indecomposable, there exists a cycle G' of G_i together with its cycle legs such that $\omega_i|_{G'} \in \tau(G')$ is indecomposable. Thus $\omega|_{G'} \in \tau(G')$ is indecomposable.

If there exists a cycle edge e with $\omega_e \in \{0, 2\}$, then let e_1 and e_2 be new leaf edges obtained by cutting G at e. The labeling $\omega \in \tau(G)$ gives a labeling $\overline{\omega} \in \tau(G^e)$ that is indecomposable. Otherwise one could lift a decomposition $\overline{\omega} = \overline{\omega}_1 + \overline{\omega}_2$ to a decomposition $\omega = \omega_1 + \omega_2$, because $(\overline{\omega_i})_{e_1} = (\overline{\omega_i})_{e_2}$. The graph G^e has first Betti number less than g. By induction, there exists a cycle G' of G^e together with cycle legs such that $\overline{\omega}|_{G'} \in \tau(G')$ is indecomposable. Thus $\omega|_{G'} \in \tau(G')$ is indecomposable. $\square$

5.4 Graphs with First Betti Number 2

We know from [BBKM11] that any minimal generator of the phylogenetic semigroup on a graph with first Betti number 2 has degree at most three. In this section, we will explicitly describe which phylogenetic semigroups have which maximal degrees of the minimal generating sets for all graphs with first Betti number 2. We will see that there are graphs with the maximal degrees of the minimal generators equal to one, two, and three. Our analysis is based on five different cases depending on the structure of the graph – whether the cycles live in different components of the graph, share at least one edge, share exactly a single vertex, there is a single edge connecting the cycles, or the cycles are more than one edge apart from each other, see Figure 5.2 for the latter four cases.

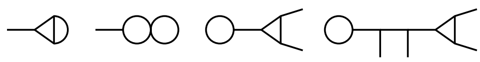


Figure 5.2: A graph with (a) cycles sharing at least one edge, (b) cycles sharing exactly a single vertex, (c) a single edge connecting cycles, (d) cycles more than one edge apart from each other

Remark. Assume a graph has a degree two vertex v. Denote the edges incident to v by e_1 and e_2. By the definition of the phylogenetic semigroup on a graph, we have $\omega_{e_1} = \omega_{e_2}$ for $\omega \in \tau(G)$. Hence, the elements of $\tau(G)$ are in one-to-one correspondence with the elements of $\tau(G')$ where G' is obtained from G by replacing e_1 and e_2 by a single edge. To simplify future analysis, from now on we will assume that graphs possess no degree two vertices.

Theorem 5.14. *Let G be a graph with first Betti number 2. The maximal degree of a minimal generator of $\tau(G)$ is*

- *one if and only if G does not contain any cycle legs that are not cycle edges;*
- *two if and only if*
  - *the cycles of G live in different connected components, or*
  - *G contains at least one cycle leg that is not a cycle edge, all cycles of G live in the same connected component, and they are not separated by an inner vertex;*
- *three if and only if the minimal cycles of G live in the same connected component and are more than one edge apart from each other;*

We will study these different cases in Lemmas 5.17–5.22. As a corollary, we can describe the minimal generating sets of the phylogenetic semigroups on those trivalent graphs with first Betti number two that do not have any minimal generators of degree three.

Corollary 5.15. *Let G be a graph with first Betti number 2 not containing any cycle legs that are not cycle edges. A labeling $\omega \in \tau(G)$ is a minimal generator of $\tau(G)$ if and only if ω is a network.*

Proof. The statement follows from Theorem 5.14 and Lemma 5.7. □

Corollary 5.16. *Let G be a trivalent graph with first Betti number 2, and*

- *the cycles of G live in different connected components, or*
- *G contains at least one cycle leg that is not a cycle edge, all cycles of G live in the same connected component, and they are not separated by an inner vertex.*

A labeling $\omega \in \tau(G)$ is a minimal generator of $\tau(G)$ if and only if it satisfies one of the following conditions:

- *ω is a network, or*
- *ω has degree two and there exists a cycle G' of G together with its cycle legs such that $\omega|_{G'} \in \tau(G')$ is indecomposable.*

Proof. The statement follows from Theorem 5.14, Lemma 5.7, and Lemma 5.13. □

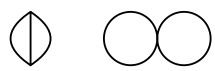


Figure 5.3: Graphs with first Betti number 2 whose phylogenetic semigroups are normal

Lemma 5.17. *Let G be a graph with first Betti number 2 that does not contain any cycle legs that are not cycle edges. The maximal degree of a minimal generator of $\tau(G)$ is one.*

Proof. The cycles of G live in the same connected component. Otherwise G would have a degree two vertex. If the connected component of G containing the cycles has one vertex, then it is isomorphic to the right graph in Figure 5.3. If the connected component of G containing the cycles has two vertices, then it is isomorphic to the left graph in Figure 5.3. The connected component of G containing the cycles cannot have three or more vertices, because every vertex must belong to at least two cycles.

By computations with `Normaliz` [BI], the phylogenetic semigroup on the left graph in Figure 5.3 is

$$\mathbb{N}\{(0,0,0,1),(1,1,0,1),(1,0,1,1),(0,1,1,1)\},$$

where the last coordinate corresponds to the degree and the first three coordinates correspond to edges of G in any fixed order.

By simple observation, the phylogenetic semigroup on the right graph in Figure 5.3 is

$$\mathbb{N}\{(0,0,1),(1,0,1),(0,1,1)\},$$

where the last coordinate corresponds to the degree and the first two coordinates correspond to edges of G in any fixed order. $\square$

Lemma 5.18. *Let G be a graph with first Betti number 2 and cycles living in different connected components. The maximal degree of a minimal generator of $\tau(G)$ is two.*

Proof. Define $\omega \in \tau(G)$ of degree two as follows: $\omega_e = 1$ for all cycle edges e of a cycle G' of G, $\omega_e = 2$ for one cycle leg of G', and $\omega_e = 0$ for all other cycle legs of G'. Extend this partial labeling of G in any feasible way to a degree two labeling of G. By Lemma 5.12, ω is indecomposable. Hence, the maximal degree of a minimal generator of $\tau(G)$ is at least two.

On the other hand, we show that every element $\omega \in \tau(G)$ can be decomposed as a sum of degree one and degree two elements. By Corollary 5.11, ω restricted to each connected component decomposes as a sum of degree one and degree two elements. These decompositions can be combined to a decomposition of $\omega \in \tau(G)$ as a sum of degree one and degree two elements. Hence, the maximal degree of a minimal generator of $\tau(G)$ is exactly 2. $\square$

We recall the notation from the previous chapter. Let G be a trivalent graph and v be an inner vertex of G. Let $\{e_1, e_2, e_3\}$ be the edges of $\Yup$ and $i_v : \Yup \hookrightarrow G$ be a map that is locally an embedding and sends the central vertex of $\Yup$ to v. For $\omega \in \tau(G)$ denote

$$a_v(\omega) := \omega_{i_v(e_1)}, \quad b_v(\omega) := \omega_{i_v(e_2)}, \quad c_v(\omega) := \omega_{i_v(e_3)}.$$

In other words, a_v, b_v, c_v measure the coefficients of ω at the edges incident to v.

Every element $\omega \in \tau(G)$ decomposes locally in a unique way into paths around an inner vertex v. This means that there exist non-negative integers $x_v(\omega)$, $y_v(\omega)$, $z_v(\omega)$ such that

$$\begin{aligned} a_v(\omega) &= y_v(\omega) + z_v(\omega), \\ b_v(\omega) &= x_v(\omega) + z_v(\omega), \\ c_v(\omega) &= x_v(\omega) + y_v(\omega), \end{aligned}$$

and $x_v(\omega) + y_v(\omega) + z_v(\omega) \leq \deg(\omega)$, see also Figure 5.4.

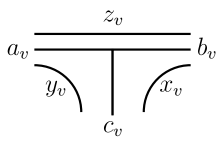


Figure 5.4: Notation for local paths at a vertex

Let T be a trivalent tree and $\omega_1, \omega_2 \in \tau(T)$ networks. Let v be an inner vertex of T. Then either $a_v(\omega_1) = a_v(\omega_2)$, $b_v(\omega_1) = b_v(\omega_2)$, or $c_v(\omega_1) = c_v(\omega_2)$, since $a_v(\omega_i) + b_v(\omega_i) + c_v(\omega_i) \in \{0, 2\}$ for $i = 1, 2$. We denote this edge by e. By exchanging values of ω_1 and ω_2 on all edges of T that are on the same side with e from v, we get $\omega_1', \omega_2' \in \tau(T)$ such that $\omega_1 + \omega_2 = \omega_1' + \omega_2'$. We call this operation *branch swapping.*

Lemma 5.19. *Let G be a graph with first Betti number 2 containing at least one cycle leg that is not a cycle edge and with two cycles sharing at least one edge. The maximal degree of a minimal generator of $\tau(G)$ is two.*

Proof. By Corollary 5.5, we can assume that G is a multiple polygon graph. There is at least one cycle leg e' of G that is not a cycle edge for any of the cycles of G. Assume that e' is a cycle leg of a cycle G'. Define ω of degree two as follows: $\omega_e = 1$ for all cycle edges e of G', $\omega_{e'} = 2$, and $\omega_e = 0$ for all other edges e of G. By Lemma 5.12, the labeling $\omega \in \tau(G)$ is indecomposable. Hence, the maximal degree of a minimal generator is at least two.

On the other hand, we show that every element $\omega \in \tau(G)$ can be decomposed as a sum of degree one and degree two elements. If G is not trivalent, then by Lemma 4.7 we can construct a trivalent graph G' with first Betti number 2 such that the maximal degree of the minimal generating set of $\tau(G)$ is less or equal than the one of $\tau(G')$. Moreover, two cycles of G' share an edge. Hence, we can assume that G is a trivalent graph.

If there is a cycle edge e of G with $\omega_e \in \{0, \deg(\omega)\}$, we construct the graph G^e with first Betti number 1 by cutting G at e. Denote the new leaf edges by e_1 and e_2. The labeling ω gives a labeling $\overline{\omega}$ of G^e. By Theorem 5.9, the labeling $\overline{\omega}$ can be decomposed as a sum of degree one and two labelings

$$\overline{\omega} = \sum_{i=1}^{\deg(\omega)} \overline{\omega_i}$$

where

$$(\overline{\omega_i})_{e_1} = (\overline{\omega_i})_{e_2} = \begin{cases} 0 & \text{if } \omega_e = 0 \\ \deg(\overline{\omega_i}) & \text{if } \omega_e = \deg(\omega) \end{cases}$$

Hence, the decomposition of $\overline{\omega}$ gives a decomposition of ω with all labelings having degree one or two. From now on we assume that there is no cycle edge e of G with $\omega_e \in \{0, \deg(\omega)\}$.

There are exactly two vertices of G incident to three cycle edges. We denote them by u and v. We construct a tree G' from G by replacing the vertex u with three new vertices u_1, u_2, and u_3 as in Figure 5.5. The labeling ω gives a labeling ω' of G'. Abusing the notation slightly, we denote by $a_u(\omega'), b_u(\omega'), c_u(\omega')$ the coordinates of ω' corresponding to leaf edges with endpoints u_1, u_2, u_3, respectively.

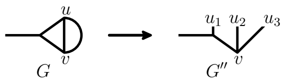


Figure 5.5: Construction of G'' from G by replacing u with u_1, u_2, u_3

The labeling ω' can be decomposed as a sum of degree one labelings

$$\omega' = \sum_{i=1}^{\deg(\omega)} \omega'_i.$$

From this we want to construct a decomposition of $\omega \in \tau(G)$. To lift an element of $\tau(G')$ to an element of $\tau(G)$, the parity and the degree condition have to be satisfied at leaf edges with endpoints u_1, u_2, u_3. This is not true for all ω'_i. We need to combine and alter these elements. We will use local paths to assure the parity and degree conditions are satisfied. We will construct the decomposition of $\omega \in \tau(G)$ iteratively. In each step, we construct a degree one or two element ω^* and then take $\omega := \omega - \omega^*$.

Case 1. $\deg_u(\omega) = \deg(\omega)$. Note that $x_u(\omega), y_u(\omega), z_u(\omega) \geq 1$, otherwise there would be a cycle edge e of G with $\omega_e = \deg(\omega)$.

- If there is ω'_i with exactly two of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1, then ω'_i can be lifted to a degree one labeling of G.
- Otherwise if there is ω'_i with exactly one of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1, then there is ω'_j with all of $a_u(\omega'_j), b_u(\omega'_j), c_u(\omega'_j)$ equal to 1. Then $\omega'_i + \omega'_j$ can be lifted to a degree two labeling of G.
- Otherwise there has to be ω'_i with all of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 0. Then there is ω'_j with all of $a_u(\omega'_j), b_u(\omega'_j), c_u(\omega'_j)$ equal to 1. After branch swapping of ω'_i and ω'_j at v, we get a labeling with exactly two values corresponding to a_u, b_u, c_u equal to 1. It can be lifted to a degree on labeling of G.

Case 2. $\deg_u(\omega) < \deg(\omega)$.

- If there exists ω'_i with $a_u(\omega'_i) = b_u(\omega'_i) = c_u(\omega'_i) = 0$, then ω'_i lifts to a labeling of $\tau(G)$.

Otherwise consider two subcases:
Case 2.1. $x_u(\omega), y_u(\omega), z_u(\omega) \geq 1$.

- If there is ω'_i with exactly two of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1, then ω'_i can be lifted to a degree one labeling of G.
- Otherwise if there is ω'_i with all of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1, then there is ω'_j with exactly one of $a_u(\omega'_j), b_u(\omega'_j), c_u(\omega'_j)$ equal to 1. Then $\omega'_i + \omega'_j$ can be lifted to a degree two labeling of G.

- Otherwise all ω'_i have exactly one of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1. Since $x_u(\omega) \geq 1$, there is ω'_i with $a_u(\omega'_i) = c_u(\omega'_i) = 0$ and $b_u(\omega'_i) = 1$, and ω'_j with $a_u(\omega'_j) = b_u(\omega'_j) = 0$ and $c_u(\omega'_j) = 1$. Then $\omega'_i + \omega'_j$ can be lifted to a degree two labeling for G.

Case 2.2. Exactly two of $x_u(\omega), y_u(\omega), z_u(\omega) \geq 1$. It is not possible to have only one $x_u(\omega), y_u(\omega), z_u(\omega) \geq 1$, because we assumed $\omega_e > 0$ for every cycle edge e. We assume that $x_u(\omega), y_u(\omega) \geq 1$, the other two cases are analogous.

- If there is ω'_i with exactly $b_u(\omega'_i), c_u(\omega'_i)$, or $a_u(\omega'_i), c_u(\omega'_i)$ equal to 1, then ω'_i can be lifted to a degree one labeling of G.

- Otherwise if there is ω'_i with exactly $a_u(\omega'_i), b_u(\omega'_i)$ equal to 1, there is ω'_j with exactly $c_u(\omega'_i)$ equal to 1, since $c_u(\omega) > a_u(\omega)$ and $c_u(\omega) > b_u(\omega)$. After branch swapping ω'_i and ω'_j at v, we either get a labeling with all values corresponding to a_u, b_u, c_u equal to 0 or a labeling with values corresponding to b_u, c_u equal to 1 or a labeling with values corresponding to a_u, c_u equal to 1. They all can be lifted to a degree one labeling of G.

- Otherwise if there is ω'_i with all of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1, there is ω'_j with exactly $c_u(\omega'_j)$ equal to 1, since $c_u(\omega) > a_u(\omega)$ and $c_u(\omega) > b_u(\omega)$. Then $\omega_i + \omega_j$ can be lifted to a degree two labeling of G.

- Otherwise all ω'_i have exactly one of $a_u(\omega'_i), b_u(\omega'_i), c_u(\omega'_i)$ equal to 1. Since $x_u(\omega) \geq 1$, there is ω'_i with $a_u(\omega'_i) = c_u(\omega'_i) = 0$ and $b_u(\omega'_i) = 1$, and ω'_j with $a_u(\omega'_j) = b_u(\omega'_j) = 0$ and $c_u(\omega'_j) = 1$. Then $\omega'_i + \omega'_j$ can be lifted to a degree two labeling for G.

At each step a degree one or two element is constructed. This assures that the iterative process comes to an end, because the degree of ω decreases. □

Lemma 5.20. *Let G be a graph with first Betti number 2 containing at least one cycle leg that is not a cycle edge and with two cycles sharing exactly one vertex. The maximal degree of a minimal generator of $\tau(G)$ is two.*

Proof. By Corollary 5.5, we can assume that G is a multiple polygon graph. There is at least one cycle leg e' of G that is not a cycle edge for any of the cycles of G. Assume that e' is a cycle leg of a cycle G'. Define ω of degree two as follows: $\omega_e = 1$ for all cycle edges e of G', $\omega_{e'} = 2$, and $\omega_e = 0$ for all other edges e of G. By Lemma 5.12, the labeling $\omega \in \tau(G)$ is indecomposable. Hence, the maximal degree of a minimal generator is at least two.

On the other hand, we show that every element $\omega \in \tau(G)$ can be decomposed as a sum of degree one and degree two elements. We construct a trivalent graph G' from G as in Lemma 4.7 such the that the maximal degree of the minimal generating set of $\tau(G)$ is less or equal than the one of $\tau(G')$. In particular, first we decrease the valency at the vertex v that is on both cycles. We replace it by vertices v', v'', and an edge e between them such that e belongs to both cycles. We repeat replacing vertices until there are only trivalent vertices left. The graph G' has two cycles that share at least one edge, thus we can apply Lemma 5.19. □

Lemma 5.21. *Let G be a graph with first Betti number 2 and the two cycles separated by a single edge e. The maximal degree of a minimal generator of $\tau(G)$ is two.*

Proof. Define $\omega \in \tau(G)$ of degree two as follows: $\omega_e = 1$ for all cycle edges e, $\omega_e = 2$ for the single edge separating cycles, and $\omega_e = 0$ for all other edges. By Lemma 5.12, ω is indecomposable. Hence, the maximal degree of a minimal generator of $\tau(G)$ is at least two.

On the other hand, we show that every element $\omega \in \tau(G)$ can be decomposed as a sum of degree one and degree two elements. If G is not trivalent, then by Lemma 4.7 we can construct a trivalent graph G' with first Betti number 2 such that the maximal degree of the minimal generating set of $\tau(G)$ is less or equal than the maximal degree of the minimal generating set of $\tau(G')$. Moreover, we may assume that every time we replace a vertex v on a cycle by vertices v', v'', and an edge between them, then v', v'' belong to the same cycle. This assures that the two cycles of G' are separated by a singe edge. Hence, we can assume that G is a trivalent graph.

Let e_1, e_2 be new leaf edges obtained by cutting G at e, and write $G^e = G_1 \sqcup G_2$. The labeling ω gives labelings ω_1 of G_1 and ω_2 of G_2. By Corollary 5.11, we can decompose ω_1 and ω_2 as a sum of degree one and degree two elements. Because all degree two labelings in these decompositions have values 0 or 2 corresponding to the edges e_1 and e_2, we can combine decompositions of ω_1 and ω_2 to get a decomposition of ω that consists of degree one and two elements. Hence, the maximal degree of a minimal generator of $\tau(G)$ is exactly two. $\square$

Lemma 5.22. *Let G be a graph with first Betti number 2 and the two cycles more than one edge apart from each other. The maximal degree of a minimal generator of $\tau(G)$ is three.*

Proof. By Corollary 5.5, we can assume that G is a multiple polygon graph. We need to specify a degree three indecomposable element $\omega \in \tau(G)$. Fix an inner vertex v on the path between the two cycles of G and an edge e^* incident to v that is not on the path between the two cycles. Define $\omega_e = 2$ for all cycle edges e and all edges e on the path between the cycles of G, $\omega_{e^*} = 2$, and $\omega_e = 0$ for all other edges e.

We will show that ω is indecomposable as a degree three labeling. By contradiction, assume $\omega = \omega_1 + \omega_2$ where $\deg(\omega_1) = 1$ and $\deg(\omega_2) = 2$. We must have $(\omega_2)_e = 1$ for all cycle edges of G and $(\omega_2)_e = 2$ for both cycle legs e that lie on the path between the two cycles. Hence, we have $(\omega_2)_e = 2$ for all edges e that lie on the path between the two cycles. Thus $(\omega_1)_{e^*} = 2$. This leads to a contradiction, because $\deg(\omega_1) = 1$. Hence, the labeling ω is a degree three indecomposable element in $\tau(G)$. $\square$

Proof of Theorem 5.14. Theorem follows from Lemmas 5.17–5.22. $\square$

5.5 Minimal Generators of Degree Three

In this section, we will describe the minimal generators of degree three of the phylogenetic semigroups on the trivalent graphs with first Betti number 2 and with the cycles more than one edge apart from each other. As a result, we can describe the minimal generating sets of the phylogenetics semigroups on the trivalent graphs with first Betti number 2 and with the cycles more than one edge apart from each other.

Theorem 5.23. *Let G be a trivalent graph with first Betti number 2 and the cycles of G more than one edge apart from each other. Then $\omega \in \tau(G)$ is a minimal generator of $\tau(G)$ if and only if it satisfies one of the following conditions:*

- *ω is a network, or*
- *ω has degree two, and there exists a cycle G' of G together with its cycle legs such that $\omega|_{G'} \in \tau(G')$ is indecomposable, or*
- *ω has degree three, and it satisfies the following three conditions:*
  - *(i) ω restricted to any cycle with its cycle legs does not decompose as a sum of degree one labelings,*
  - *(ii) ω restricted to an edge on the shortest path between two cycles has value one or two, and*
  - *(iii) ω restricted to exactly one edge incident to an edge on the shortest path between two cycles that is not a cycle edge or an edge on the shortest path has value one or two, and has value zero or three on all other such edges.*

Together with Corollaries 5.15 and 5.16, Theorem 5.23 completes the characterization of the minimal generating sets of the phylogenetic semigroups on the trivalent graphs with first Betti number 2.

This section is organized as follows. In Lemma 5.24, we will characterize when a degree three labeling on a trivalent polygon graph cannot be decomposed as a sum of degree one labelings, and then we will extend this characterization to all trivalent graphs with first Betti number 1 in Corollary 5.26. In Lemma 5.27, we will use these results to describe the indecomposable labelings of degree three on the trivalent graphs with first Betti number 2 and cycles more than one edge apart from each other.

Let G be a trivalent graph with first Betti number 1 and ω a degree two indecomposable labeling. Label the cycle legs of G where ω has value two by $e_0, \dots, e_{2k}$ in clockwise order. Slightly abusing the notation, we write e_{i+j} for $e_{i+j \mod 2k}$ where $i + j > 2k$. Label by $P_{e',e''}$ the path starting at a cycle leg e' and going in the clockwise direction until reaching a cycle leg e'' . Write P_i for $P_{e_i,e_{i+1}}$. We say a cycle leg e is between cycle legs e_i and e_j, when e is between cycle legs e_i and e_j in clockwise direction.

Lemma 5.24. *Let G be a trivalent polygon graph and $\omega \in \tau(G)$ a degree three labeling. Then ω cannot be decomposed as a sum of degree one labelings if and only if $\omega = \omega_1 + \omega_2$ such that*

- $\deg(\omega_1) = 1$ *and* $\deg(\omega_2) = 2$*,*
- *ω_2 is indecomposable with value two on cycle legs $e_0, \dots, e_{2k}$ and value zero on all other cycle legs,*

- ω_1 *is* $P_0 \cup P_2 \cup \ldots \cup P_{2k-2}$, $P_0 \cup P_2 \cup \ldots P_{2k-4} \cup P_{e_{2k-2},e_{2k}}$, *or* $P_0 \cup P_2 \cup \ldots P_{2k-2} \cup P_{e_{2k},e'}$ *where* e' *is a cycle leg between* e_{2k} *and* e_0, *or also the cycle path if* $k = 0$.

Proof. A degree three labeling ω can be always decomposed as $\omega = \omega_1 + \omega_2$ with $\deg(\omega_1) = 1$ and $\deg(\omega_2) = 2$. We show that unless ω_1, ω_2 are as in the statement of the lemma, we can alter ω_1, ω_2 to get ω_1', ω_2' such that $\omega_1 + \omega_2 = \omega_1' + \omega_2'$ and ω_2' decomposes as a sum of two degree one labelings.

If there is P_i such that it does not intersect the network ω_1, then the union of ω_1 and P_i is a network and the complement of P_i in ω_2 decomposes as the sum of $P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{i-2}$ and $P_{i+2} \cup P_{i+4} \cup \ldots \cup P_{i-1}$. We will assume from now on that every P_i intersects ω_1.

If there exist e_i and e_j such that neither of them is incident to a path in ω_1, then either $e_j = e_{i+2l}$ or $e_i = e_{j+2l}$ for some $1 \leq l \leq k$. In the first case, let Γ be the union of paths in ω_1 from e_i to e_j, and define $\omega_1' = \omega_1 \backslash \Gamma \cup P_i \cup P_{i+2} \cup \ldots \cup P_{j-2}$ and $\omega_2' = \omega_2 \backslash (P_i \cup P_{i+2} \cup \ldots \cup P_{j-2}) \cup \Gamma$. Then ω_2' decomposes as the sum $\Gamma \cup P_j \cup P_{j+2} \cup \ldots \cup P_{i-1}$ and $P_{j+1} \cup P_{j+3} \cup \ldots \cup P_{i-2} \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{j-1}$. In the second case, the same discussion applies for i and j exchanged. We will assume from now on that there is at most one e_i that is not incident to a path in ω_1.

If ω_1 corresponds to the cycle path P_{cycle} and $k \geq 1$, then ω decomposes as the sum of P_{e_2,e_1} and $P_{e_0,e_2} \cup P_3 \cup P_5 \cup \ldots \cup P_{2k-1}$ and $P_{e_1,e_3} \cup P_4 \cup P_6 \cup \ldots \cup P_{2k}$. Here we use that $P_{\text{cycle}} \cup P_0 \cup P_1 \cup P_2 = P_{e_0,e_2} \cup P_{e_1,e_3} \cup P_{e_2,e_1}$.

It there is a path $P_{e',e''}$ in ω_1 such that not both e', e'' belong to $\{e_0, \ldots, e_{2k}\}$, then we consider five different cases:

- If there is a path P_i such that e', e'' are both between e_i and e_{i+1}, define $\omega_1' = \omega_1 \backslash P_{e',e''}$ and $\omega_2'' = \omega_2 \cup P_{e',e''}$. Since $P_{e',e''} \cup P_i = P_{e_i,e''} \cup P_{e',e_{i+1}}$, the labeling ω_2' decomposes as the sum of $P_{e_i,e''} \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{i-2}$ and $P_{e',e_{i+1}} \cup P_{i+2} \cup P_{i+4} \cup \ldots \cup P_{i-1}$.

- If there is a path P_i such that e' is before e_i and e'' is between e_i and e_{i+1}, define $\omega_1' = \omega_1 \backslash P_{e',e''} \cup P_{e',e_i}$ and $\omega_2' = \omega_2 \backslash (P_{i-1} \cup P_i) \cup P_{e_{i-1},e_{i+1}} \cup P_{e_i,e''}$. Then $\omega_1 + \omega_2 = \omega_1' + \omega_2'$, since $P_{e',e''} \cup P_{i-1} \cup P_i = P_{e',e_i} \cup P_{e_{i-1},e_{i+1}} \cup P_{e_i,e''}$. Then ω_2' decomposes as the sum of $P_{e_{i-1},e_{i+1}} \cup P_{i+2}, \ldots \cup P_{i-3}$ and $P_{e_i,e''} \cup P_{i+1} \cup \ldots \cup P_{i-2}$.

- If there are paths $P_{e_i,e'}$ and P_{e'',e_j} in ω_1 such that e' is between e_i and e_{i+1}, and e'' is between e_{j-1} and e_j, and $e_j = e_{i+2l+1}$ for some $0 \leq l \leq k-1$, let Γ be the union of paths between e_i and e_j. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_i \cup P_{i+2} \cup \ldots \cup P_{j-1}$ and $\omega_2' = \omega_2 \backslash (P_i \cup P_{i+2} \cup \ldots \cup P_{j-1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $P_{e_i,e'} \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{i-2}$ and $\Gamma \backslash P_{e_i,e'} \cup P_{j+1} \cup P_{j+3} \cup \ldots \cup P_{i-1}$.

- If there are paths $P_{e_i,e'}$ and P_{e'',e_j} in ω_1 such that the edge e' is between e_i and e_{i+1}, the edge e'' is between e_{j-1} and e_j and $e_j = e_{i+2l}$ for some $1 \leq l \leq k$, let Γ be the union of paths between e_j and e_i together with $P_{e_i,e'}$ and P_{e'',e_j}. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_j \cup P_{j+2} \cup \ldots \cup P_{i-1}$ and $\omega_2' = \omega_2 \backslash (P_j \cup P_{j+2} \cup \ldots \cup P_{i-1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $\Gamma \backslash P_{e_i,e'} \cup P_i \cup P_{i+2} \cup \ldots \cup P_{j-2}$ and $P_{e_i,e'} \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{i-2}$.

- If there are paths $P_{e_i,e'}$ and $P_{e_j,e''}$ in ω_1 such that the edge e' is between e_i and e_{i+1}, the edge e'' is between e_j and e_{j+1} and $e_j = e_{i+2l}$ for some $1 \le l \le k$, let Γ be the union of paths in ω_1 between e_i and e'' without $P_{e_i,e'}$. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{j-1}$ and $\omega_2' = \omega_2 \backslash (P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{j-1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $P_{e_j,e''} \cup P_{j+1} \cup P_{j+3} \cup \ldots \cup P_{j-2}$ and $P_j \cup P_{j+2} \cup \cdots \cup P_{i-1} \cup \Gamma \backslash P_{e_j,e''}$. If $e_j = e_{i+2l+1}$ for some $0 \le l \le k-1$ then the same discussion works for i and j exchanged.

If none of the five if-conditions holds, then the unique path of the form $P_{e',e''}$ in ω_1 such that not both e', e'' belong to $\{e_0, \ldots, e_{2k}\}$ must be $P_{e_i,e'}$ or $P_{e'',e_{i+1}}$ with $e,' e''$ between e_i and e_{i+1}.

If there is a path in ω_1 of the form P_{e_i,e_j}, then we consider three different cases:

- If there exists P_{e_i,e_j} with $e_j = e_{i+2l+1}$ for $1 \le l \le k-1$, then define $\omega_1' = \omega_1 \backslash P_{e_i,e_j} \cup P_i \cup P_{i+2} \cup \ldots \cup P_{j-1}$ and $\omega_2' = \omega_2 \backslash (P_i \cup P_{i+2} \cup \ldots \cup P_{j-1}) \cup P_{e_i,e_j}$. Since $P_{e_i,e_j} \cup P_{j-2} = P_{e_i,e_{j-1}} \cup P_{e_{j-2},e_j}$, then ω_2' decomposes as the sum of $P_{e_i,e_{j-1}} \cup P_j \cup P_{j+2} \cup \ldots \cup P_{i-2}$ and $P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{j-4} \cup P_{e_{j-2},e_j} \cup P_{j+1} \cup P_{j+3} \cup \ldots \cup P_{i-1}$.

- If there exists P_{e_i,e_j} with $e_j = e_{i+2l}$ for $2 \le l \le k$, assume that $j = 0$. Define $\omega_1' = \omega_1 \backslash P_{e_i,e_j} \cup P_{e_i,e_{j-2}} \cup P_{j-1}$ and $\omega_2' = \omega_2 \backslash (P_{j-3} \cup P_{j-2} \cup P_{j-1}) \cup P_{j-3,j-1} \cup P_{j-2,j}$. Then $\omega_1 + \omega_2 = \omega_1' + \omega_2'$ since $P_{e_i,e_j} \cup P_{j-3} \cup P_{j-2} \cup P_{j-1} = P_{e_i,e_{j-2}} \cup P_{j-3,j-1} \cup P_{j-2,j} \cup P_{j-1}$. Then ω_2' decomposes as the sum of $P_0 \cup P_2 \cup \ldots \cup P_{j-3,j-1}$ and $P_1 \cup P_3 \cup \ldots \cup P_{j-2,j}$.

- If there exist $P_{e_{i_1},e_{i_2}}, P_{e_{j_1},e_{j_2}}$ such that $e_{i_2} = e_{i_1+2l}, e_{j_2} = e_{j_1+2m}$ for $1 \le l, m \le k$ and $e_{j_2} = e_{i_1+2n+1}$ for some $0 \le n \le k-1$, assume that P_{j_1,j_2} is the next path with such property after P_{i_1,i_2} in clockwise direction. Denote all paths between e_{i_1} and e_{j_2} in ω_1 by Γ. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_{i_1} \cup P_{i_1+2} \cup \ldots \cup P_{j_2-1}$ and $\omega_2' = \omega_2 \backslash (P_{i_1} \cup P_{i_1+2} \cup \ldots \cup P_{j_2-1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $\Gamma \backslash\ P_{e_{j_1},e_{j_2}} \cup P_{j_1} \cup P_{j_1+2} \cup \cdots \cup P_{i_1-2}$ and $P_{i_1+1} \cup P_{i_1+3} \cup \ldots \cup P_{j_1-2} \cup P_{e_{j_1},e_{j_2}} \cup P_{j_2+1} \cup \ldots \cup P_{i_1-1}$. If $e_{j_2} = e_{i_1+2n}$ for some $1 \le n \le k-1$ then the same discussion works for i's and j's exchanged.

If none of the three if-conditions holds, then only paths in ω_1 of the form P_{e_i,e_j} can be P_i, and at most one $P_{e_j,e_{j+2}}$.

Finally, we have to show that ω_1 cannot simultaneously contain paths $P_{e_i,e'}$ and $P_{e_j,e_{j+2}}$ where $i, j \in \{0, \ldots, 2k\}$ and e' is between e_i and e_{i+1}. We consider two different cases: $e_j = e_{i+2l}$ for $1 \le l \le k-1$ and $e_j = e_{i+2l+1}$ for $0 \le l \le k-1$. If we have P_{e',e_i} instead of $P_{e_i,e'}$ then we can apply the same discussion in the counterclockwise direction.

In the first case there must be e_t with $t = i + 2l + 1$ between e' and e_j that is not incident to any of the paths in ω_1. Otherwise paths between e' and e_j in ω_1 would be $P_{i+1}, P_{i+3}, \ldots, P_{j-1}$, which is not possible, since $P_{e_j,e_{j+2}}$ is in ω_1. Let Γ be the union of paths in ω_1 between e_i and e_t. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_i \cup P_{i+2} \cup \ldots \cup P_{t-1}$ and $\omega_2' = \omega_2 \backslash (P_i \cup P_{i+2} \cup \ldots \cup P_{t-1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $\Gamma \cup P_t \cup P_{t+2} \cup \ldots P_{i-2}$ and $P_{t+1} \cup P_{t+3} \cup \ldots P_{t-2}$.

In the second case let Γ be the union of paths in ω_1 from e_i to e_{j+2}. Define $\omega_1' = \omega_1 \backslash \Gamma \cup P_i \cup P_{i+2} \cup \ldots \cup P_{j+1}$ and $\omega_2' = \omega_2 \backslash (P_i \cup P_{i+2} \cup \ldots \cup P_{j+1}) \cup \Gamma$. Then ω_2' decomposes as the sum of $P_{e_i,e'} \cup P_{i+1} \cup P_{i+3} \cup \ldots \cup P_{i-2}$ and $\Gamma \backslash P_{e_i,e'} \cup P_{j+3} \cup P_{j+5} \cup \ldots \cup P_{i-1}$.

If none of the previous is true for ω, then ω is as in the statement of the lemma. We will show that the only decomposition of ω is $\omega = \omega_1 + \omega_2$. This implies that we cannot decompose ω as a sum of degree one labelings as ω_2 is indecomposable.

In all four cases, we have $\omega_e \geq 2$ for a cycle leg e if and only if $e \in \{e_0, \ldots, e_{2k}\}$. Moreover, $\omega_{\overline{e}} = 2$ holds for at most one $\overline{e} \in \{e_0, \ldots, e_{2k}\}$. We construct a decomposition $\omega = \omega_1' + \omega_2'$ with $\deg(\omega_1') = 1$ and $\deg(\omega_2') = 2$. If $\omega_1 = P_0 \cup P_2 \cup \ldots P_{2k-2} \cup P_{e_{2k},e'}$, then $(\omega_2')_e = 2$ for all $e \in \{e_0, \ldots, e_{2k}\}$ and $(\omega_2')_e = 0$ for all other cycle legs. Indeed, there is only one cycle leg e' left with value one, but since the sum of values on all leaf edges must be even we have $(\omega_2')_{e'} = 0$. For the other three cases, $(\omega_2')_e = 2$ for all $e \in \{e_0, \ldots, e_{2k}\} \backslash \overline{e}$, since $\omega_e = 3$ for $e \in \{e_0, \ldots, e_{2k}\} \backslash \overline{e}$. Thus also $(\omega_2')_{\overline{e}} = 2$, since the sum of values on all leaf edges must be even. It follows that $(\omega_2')_e = 1$ for all cycle edges, hence $\omega_i' = \omega_i$ for $i \in \{1, 2\}$. $\square$

Corollary 5.25. *Let G be a polygon graph and $\omega \in \tau(G)$ a degree three labeling. Then ω cannot be decomposed as a sum of degree one labelings if and only if ω can be decomposed uniquely as $\omega = \omega_1 + \omega_2$ with $\deg(\omega_1) = 1$ and $\deg(\omega_2) = 2$.*

Corollary 5.26. *Let G be a trivalent graph with first Betti number 1 and $\omega \in \tau(G)$ a degree three labeling. Then ω cannot be decomposed as a sum of degree one labelings if and only if $\omega = \omega_1 + \omega_2$ such that*

- $\deg(\omega_1) = 1$ *and* $\deg(\omega_2) = 2$,
- *ω_2 is indecomposable with value two on cycle legs $e_0, \ldots, e_{2k}$ and value zero on all other cycle legs,*
- *ω_1 restricted to the unique cycle with its cycle legs is $P_0 \cup P_2 \cup \ldots \cup P_{2k-2}$, $P_0 \cup P_2 \cup \ldots P_{2k-4} \cup P_{e_{2k-2},e_{2k}}$, or $P_0 \cup P_2 \cup \ldots P_{2k-4} \cup P_{e_{2k-2},e'}$ where e' is a cycle leg between e_{2k-2} and e_{2k-1}, or also the cycle path if $k = 0$.*

Proof. The statement follows directly from Lemmas 5.24 and 5.5. $\square$

Lemma 5.27. *Let G be a trivalent graph with first Betti number 2 and the cycles of G more than one edge apart from each other. A labeling $\omega \in \tau(G)$ of degree three is indecomposable if and only if the following conditions are fulfilled:*

(i) *ω restricted to any cycle with its cycle legs does not decompose as a sum of degree one labelings,*

(ii) *ω restricted to an edge on the shortest path between two cycles has value one or two,*

(iii) *ω restricted to exactly one edge incident to an edge on the shortest path between two cycles that is not a cycle edge or an edge on the shortest path has value one or two, and has value zero or three on all other such edges.*

Proof. By Lemma 5.5, we can assume that G is a multiple polygon graph. Depict the edges on the shortest path between the two cycles horizontally and edges incident to them vertically below them as in Figure 5.2 (c).

Assume ω restricted to a cycle G_1 together with its cycle legs decomposes as a sum of degree one elements. Let e be a cycle leg of G_1 on the shortest path between G_1 and the other cycle. Write $G^e = G_1 \sqcup G_2$. Then ω decomposes on G_2, and this decomposition can be extended to G.

Assume there is an edge $\overline{e}$ on the shortest path between two cycles of G such that $\omega_{\overline{e}} \in \{0, 3\}$. Let e', e'' be new leaf edges obtained by cutting G at e, and write $G^{\overline{e}} = G' \sqcup G''$. Then $\omega|_{G'}$ and $\omega|_{G''}$ can be decomposed as

$$\omega|_{G'} = \omega'_1 + \omega'_2 \text{ and } \omega|_{G''} = \omega''_1 + \omega''_2$$

with $\deg(\omega'_1) = \deg(\omega''_1) = 1$ and $\deg(\omega'_2) = \deg(\omega''_2) = 2$. Furthermore, $(\omega'_i)_{e'} = (\omega''_i)_{e''}$ for $i = 1, 2$ and hence they can be combined to a decomposition of ω.

Assume now that the conditions $(i), (ii)$ are fulfilled. The labeling ω can be decomposed if and only if it can be decomposed as

$$\omega = \omega_1 + \omega_2$$

with $\deg(\omega_1) = 1$ and $\deg(\omega_2) = 2$. There is a unique way of defining ω_1 and ω_2 on cycles and cycle legs by Corollary 5.25. We try to construct a decomposition of ω on all other edges step-by-step going from left to right such that the decomposition is compatible with the decomposition on the cycle legs on the shortest path between the two cycles, and study when there exists no such decomposition. Let e be the leftmost edge of the shortest path between two cycles where ω_1 and ω_2 are defined, and let the vertex v be the right endpoint of e. Using the notation from Chapter 4, we want to define $b_v(\omega_i)$ and $c_v(\omega_i)$ given $a_v(\omega_i)$ for $i = 1, 2$.

All possible local decompositions of ω at an inner vertex between the two cycles (assuming that horizontal edges have values one or two) are presented in Figures 5.6 and 5.7. In Figure 5.6 the value of ω at the vertical edge is zero or three. In Figure 5.7 the value of ω at the vertical edge is one or two.

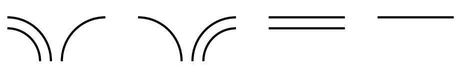


Figure 5.6: Degree three local decompositions, 1

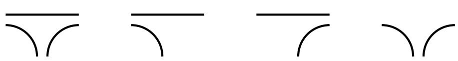


Figure 5.7: Degree three local decompositions, 2

Given a local decomposition at v as in Figure 5.6 and $a_v(\omega_i)$, then there is a unique way of defining $b_v(\omega_i)$ and $c_v(\omega_i)$. In particular, if $a_v(\omega_2) \in \{0, 2\}$ then $b_v(\omega_2) \in \{0, 2\}$. If

$a_v(\omega_2) = 1$ then $b_v(\omega_2) = 1$. Given a local decomposition at v as in Figure 5.7 and $a_v(\omega_i)$, then there might be a unique way of defining $b_v(\omega_i)$ and $c_v(\omega_i)$, or not, depending on the value of $a_v(\omega_2)$. If $a_v(\omega_2) \in \{0, 2\}$ then $b_v(\omega_2) = 1$. If $a_v(\omega_2) = 1$ then one can define either $b_v(\omega_2) \in \{0, 2\}$ or $b_v(\omega_2) = 1$.

Let e be a cycle leg that is on the path between two cycles. If $\omega_e = 2$, then $(\omega_1)_e = 0$ and $(\omega_2)_e = 2$, because a degree two indecomposable element on a cycle can have only values zero and two on cycle legs by Theorem 5.9. If $\omega_e = 1$, then $(\omega_e)_1 = 1$ and $(\omega_e)_2 = 0$ for the same reasons. Denote by e_r the cycle leg of the right cycle that are on the path between two cycles.

If the horizontal path contains labelings only as in Figure 5.6, then $b_v(\omega_2) \in \{0, 2\}$ for every vertex v on the horizontal path. In particular, $(\omega_2)_{e_r} \in \{0, 2\}$, hence there exists a decomposition of ω.

If at more than one vertex the local decomposition is as in Figure 5.7, denote the first such vertex by v' and the last one by v''. For all the vertices v left from v', the value $b_v(\omega) \in \{0, 2\}$ is uniquely defined. For v', we have $b_{v'}(\omega) = 1$. For all the vertices v between v' and v'', we can define $b_v(\omega) = 1$: If the local decomposition at v is as in Figure 5.7 then we have this choice by the discussion below. If the local decomposition at v is as in Figure 5.6 then $b_v(\omega_2) = 1$ since $a_v(\omega_2) = 1$ again by the discussion above. For $v = v''$, we define $b_v(\omega_2) \in \{0, 2\}$. At all vertices v to the right of v'', we have local decompositions as in Figure 5.6, therefore $b_v(\omega_2) \in \{0, 2\}$. In particular, $(\omega_2)_{e_r} \in \{0, 2\}$ and the decomposition of ω on the horizontal path is compatible with the decompositions of ω on both cycles. Hence, the labeling ω is decomposable.

On the other hand, if at one vertex v' the local decomposition is as in Figure 5.7 and at all other vertices the local decomposition is as in Figure 5.6, then $b_v(\omega_2) \in \{0, 2\}$ for all vertices v left from v' and $b_v(\omega_2) = 1$ for all vertices v to the right of v' including v' itself. In particular, $(\omega_2)_{e_r} = 1$ which is not compatible with the values of ω_2 on the right cycle. Since all steps have been uniquely determined, then ω cannot be decomposed. This completes the proof. □

Proof of Theorem 5.23. The statement follows from Lemmas 5.7, 5.13, and 5.27. □

5.6 Examples

In this section, we will list some examples of graphs with first Betti number 3, 4, and 5 together with the maximal degree of the minimal generating set of their phylogenetic semigroup.[1] Maximal degrees have been computed with `Normaliz` [BI]. We will also show that, for any natural number g, there exists a graph G with first Betti number g such that the maximal degree of a minimal generator of $\tau(G)$ is one.

We note that the maximal degree tends to depend on the "separateness" of the cycles, exactly as we proved in Section 5.4 for the graphs with first Betti number 2. This suggests

[1] We thank Christopher Manon for introducing us the trivalent graph with first Betti number 4 and maximal degree one, see Figure 5.10.

that the maximal degree of the minimal generating set of the phylogenetic semigroup on the g-caterpillar graph is maximal among the graphs with first Betti number g and that, for g odd, there is no graph with first Betti number g such that the maximal degree of its phylogenetic semigroup is $g+1$.

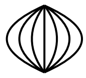


Figure 5.8: Graph with two vertices and seven edges

Example 5.28. Let G be the graph with first Betti number g that has two vertices and $g+1$ edges between the two vertices, as illustrated in Figure 5.8. Then $\tau(G)$ is generated in degree one. By cutting all edges of G, we get two claw trees T', T'' with $g+1$ leaves. Let $\omega \in \tau(G)$ be a degree d labeling. Then ω gives $\omega' \in T'$ and $\omega'' \in T''$ with $\omega' = \omega''$ that we can decompose as a sum of d degree one labelings exactly the same way on both trees. Gluing the decompositions of ω' and ω'' gives a decomposition of ω as a sum of degree one labelings.

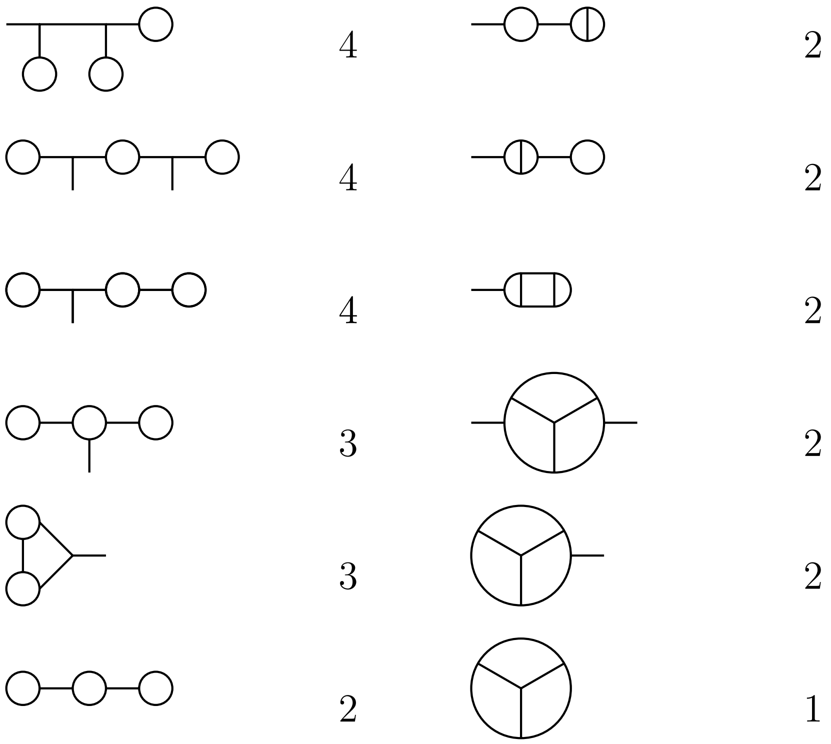


Figure 5.9: Maximal degrees of the minimal generating set of $\tau(G)$ where G is a graph with first Betti number 3

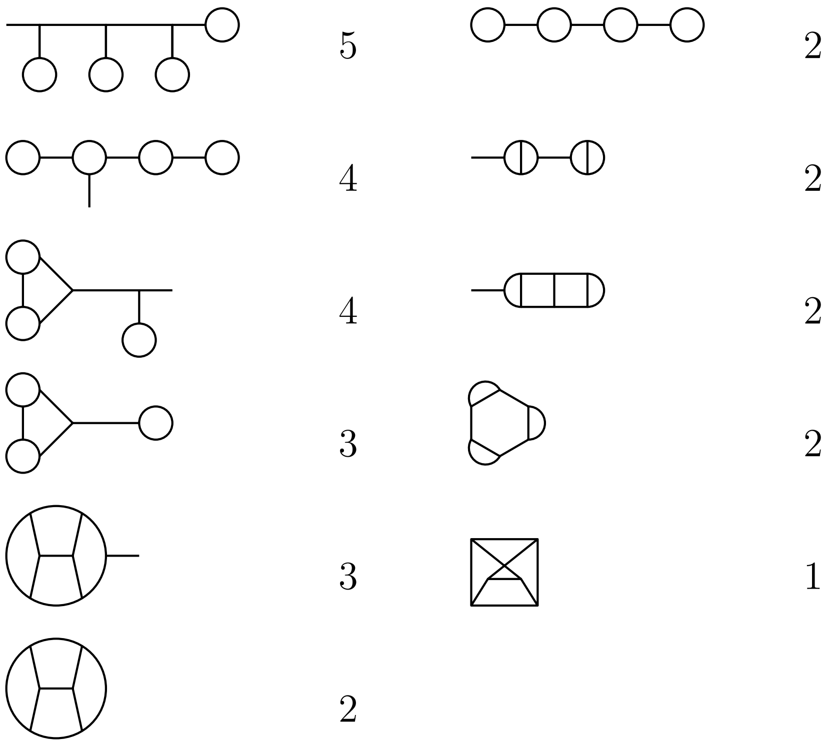


Figure 5.10: Maximal degrees of the minimal generating set of $\tau(G)$ where G is a graph with first Betti number 4

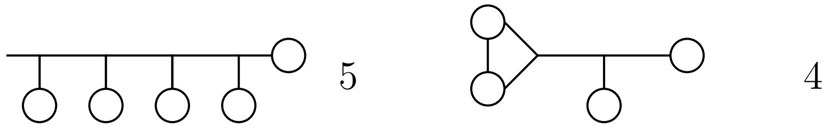


Figure 5.11: Maximal degrees of the minimal generating set of $\tau(G)$ where G is a graph with first Betti number 5

Chapter 6

Group-Based Models and Berenstein-Zelevinsky Triangles

6.1 Introduction

This chapter will be a part of a joint paper with Christopher Manon. All results presented here unless otherwise stated were worked out by the author of this dissertation independently.

The aim of this chapter is to establish a combinatorial connection between semigroups associated with group-based models and BZ triangles motivated by the work of Sturmfels, Xu and Manon. Manon constructed flat degenerations of the algebra of $\mathrm{SL}_2(\mathbb{C})$ conformal blocks for a stable curve of genus g and n marked points to the semigroup algebra of the phylogenetic semigroup on a graph with first Betti number g with n leaves [Man09]. The $g = 0$ case was first treated by Sturmfels and Xu [SX10], whereby in this case the phylogenetic semigroups are the semigroups associated with the Jukes-Cantor binary model.

Manon also constructed toric degenerations of $\mathrm{SL}_3(\mathbb{C})$ conformal block algebras to semigroup algebras of rank two graded BZ triangles [Man12a]. Berenstein and Zelevinsky defined BZ triangles as an alternative to the Littlewood-Richardson rule for counting the dimension of the triple tensor product invariants [BZ92]. BZ triangles appear for example in the work of Knutson and Tao [KT99], where they prove the saturation conjecture for the monoid of triples with the corresponding triple tensor product non-empty. From the result of Manon follows that the Hilbert polynomial of rank two graded BZ triangles associated with a trivalent tree does not depend on the shape of the tree.[1] Hence, rank two graded BZ triangles generalize the theorem by Buczyńska and Wiśniewski [BW07], which fails to be true for other group-based models [Kub12, DM12].

Therefore, semigroup algebras of the Jukes-Cantor binary model and rank two graded Berenstein-Zelevinski triangles are both toric degenerations of conformal block algebras. Their Hilbert polynomials do not depend on the shape of the tree. This raises the question

[1] We proved the same result based on Lemma 2.6 using `Macaulay2`, but as our proof relies on comparing big files containing Hilbert series we will not present it in this dissertation.

whether there is a connection between group-based models and BZ triangles. The main result of this chapter states that the semigroup associated with the group-based model with the underlying group $\mathbb{Z}_{r+1}$ is contained in the projection of the semigroup of rank r Berenstein-Zelevinsky triangles to the corresponding highest weights.

In Section 6.2, we recall the definition of a BZ triangle and the semigroup of BZ triangles on a trivalent tree. In Section 6.3, we establish the connection between group-based models and BZ triangles on trees.

6.2 BZ Triangles

Let $\mathfrak{g} = \mathfrak{sl}_{r+1}(\mathbb{C})$. Let V_λ, V_μ, V_ν be irreducible finite-dimensional $\mathfrak{g}$-modules with highest weights λ, μ, ν. The Littlewood-Richardson rule determines the dimension of the space of triple tensor product invariants $c_{\lambda\mu\nu} = \dim(V_\lambda \otimes V_\mu \otimes V_\nu)^{\mathfrak{g}}$, see for example [FH91]. In [BZ92] Berenstein and Zelevinsky gave an alternative to the Littlewood-Richardson rule. They showed that $c_{\lambda\mu\nu}$ equals the number of integer points in the intersection of a polyhedral cone with an affine subspace. These integer points are called BZ triangles. Manon and Zhou extended this definition to BZ triangles on trivalent trees [MZ12]. We will recall the definition of BZ triangles and the projections to corresponding highest weights as in [BZ92, Section 2], and then define BZ triangles on trees similarly to [MZ12, Definition 2.2].

Let T_r be the set of integer points in the triangle with the vertices $(2r-1, 0, 0), (0, 2r-1, 0)$, and $(0, 0, 2r-1)$:

$$T_r = \{(i, j, k) \in \mathbb{Z}^3 : i + j + k = 2r - 1\}.$$

Let H_r be the subset of T_r with all coordinates odd and G_r be the subset of T_r with exactly one coordinate odd:

$$\begin{aligned} H_r &= \{(i, j, k) \in T_r : \text{ all } i, j, k \text{ are odd}\}, \\ G_r &= T_r - H_r. \end{aligned}$$

Geometrically, the elements of G_r correspond to the vertices of a graph consisting of hexagons and triangles, and the elements of H_r correspond to the centers of the hexagons, see Figure 6.1.

Let $\alpha = (1, -1, 0), \beta = (0, 1, -1)$, and $\gamma = (-1, 0, 1)$. Let L_r be the subspace of $\mathbb{R}^{G_r}$ defined by the equations

$$x(\eta + \alpha) - x(\eta - \alpha) = x(\eta + \beta) - x(\eta - \beta) = x(\eta + \gamma) - x(\eta - \gamma) \tag{6.1}$$

for all $\eta \in H_r$. Geometrically, the elements of L_r correspond to the labelings of the vertices of the aforementioned graph such that $x(\xi_1) + x(\xi_2) = x(\xi'_1) + x(\xi'_2)$ for all opposite pairs of edges $[\xi_1, \xi_2]$ and $[\xi'_1, \xi'_2]$ of all hexagons. Define a polyhedral cone $K_r = L_r \cap \mathbb{R}^{G_r}_{\geq 0}$ and an affine semigroup $BZ_r = K_r \cap \mathbb{Z}$.

Definition 6.1. The elements of the affine semigroup BZ_r are called *BZ triangles*.

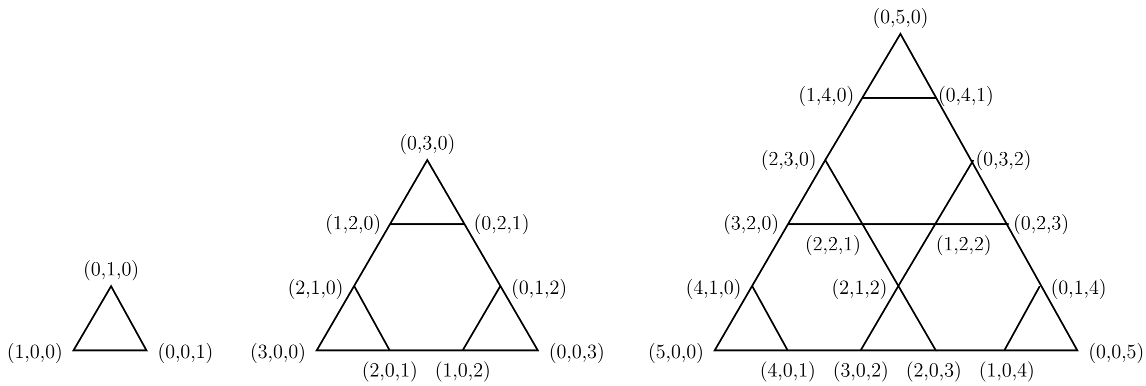


Figure 6.1: Graphs consisting of hexagons and triangles for $r = 1, 2, 3$

Remark. Affine semigroups BZ_r are numbered by the rank. In the next section, this will cause a difference by one in the numbering of the semigroups associated with rank r BZ triangles and the semigroups associated with the group-based model with group $\mathbb{Z}_{r+1}$. We stick to the numbering by rank to be consistent with [BZ92].

Example 6.2. The minimal generating sets for BZ_1 and BZ_2 are listed in Figures 6.2 and 6.3, respectively.

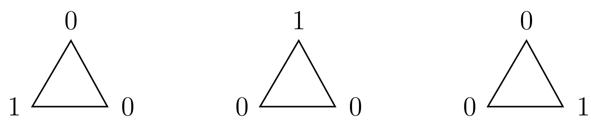


Figure 6.2: The minimal generating set for BZ_1

We identify the lattice of $\mathfrak{g}$-weights with the standard lattice $\mathbb{Z}^r$ using as the standard basis the fundamental weights $\omega_1 = (1, 0, 0, \dots, 0), \omega_2 = (1, 1, 0, \dots, 0), \dots, \omega_r = (1, 1, 1, \dots, 1)$. Define a linear projection pr:$L_r \longrightarrow \mathbb{R}^{3r}$ to the vector space of triples of $\mathfrak{g}$-weights by

$$\text{pr}(x) = (l_1, \dots, l_r; m_1, \dots, m_r; n_1, \dots, n_r)$$

where

$$\begin{aligned} l_i &= x(2(r-i)+1, 2(i-1), 0) + x(2(r-i), 2i-1, 0), \\ m_i &= x(0, 2(r-i)+1, 2(i-1)) + x(0, 2(r-i), 2i-1), \\ n_i &= x(2(i-1), 0, 2(r-i)+1) + x(2i-1, 0, 2(r-i)) \end{aligned}$$

for $i \in 1, \dots, r$. The coordinates of $\text{pr}(x)$ are pairwise sums of neighboring labels on the boundary of the triangle starting from the lower left corner and going clockwise around the triangle. In particular, the coordinates l_i correspond to the northwest edge, m_i to the northeast edge, and n_i to the south edge of the triangle.

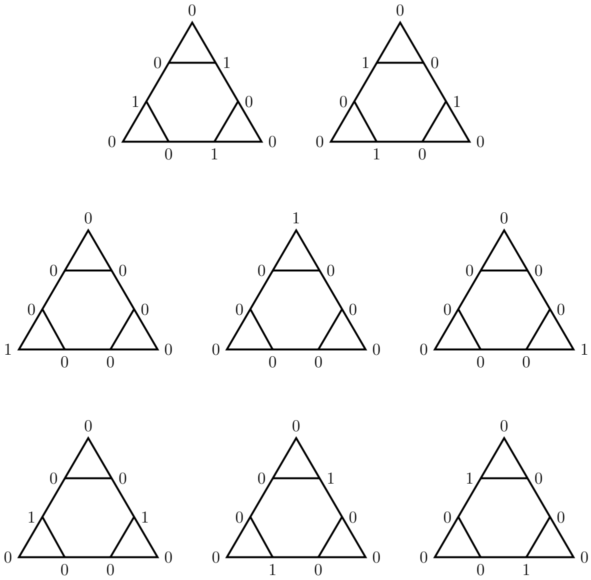


Figure 6.3: The minimal generating set for BZ_2

Example 6.3. The projections of the minimal generators of BZ_1 as in Figure 6.2 are

$$(1;0;1),(1;1;0),(0;1;1).$$

The projections of the minimal generators of BZ_2 as in Figure 6.3 are

$$\begin{gathered}(1,0;1,0;1,0),(0,1;0,1;0,1),\\(1,0;0,0;0,1),(0,1;1,0;0,0),(0,0;0,1;1,0),\\(1,0;0,1;0,0),(0,0;1,0;0,1),(0,1;0,0;1,0).\end{gathered}$$

Theorem 6.4 ([BZ92], Theorem 1)**.** *Let $\lambda=\sum l_i\omega_i$, $\mu=\sum m_i\omega_i$, and $\nu=\sum n_i\omega_i$ be three highest $\mathfrak{g}$-weights. Then the triple multiplicity $c_{\lambda\mu\nu}$ equals $|BZ_r\cap \mathrm{pr}^{-1}(\lambda,\mu,\nu)|$.*

Furthermore, we define a linear projection $\mathrm{pr}_e : L_r \longrightarrow \mathbb{R}^r$ to the vector space of $\mathfrak{g}$-weights for each edge e of the triangle by

$$\mathrm{pr}_e(x)=\begin{cases}(l_1,\dots,l_r) & \text{if } e \text{ is the northwest edge of the triangle,}\\(m_1,\dots,m_r) & \text{if } e \text{ is the northeast edge of the triangle,}\\(n_1,\dots,n_r) & \text{if } e \text{ is the south edge of the triangle.}\end{cases}$$

Then pr_e maps a BZ triangle to the corresponding λ,μ, or ν. Define $\mathrm{pr}_e^* : L_r \longrightarrow \mathbb{R}^r$ to be equal to pr_e with coordinates in the reversed order.

Now we define the affine semigroup of rank r BZ triangles on a trivalent tree similarly to [MZ12]. Given any trivalent tree T, consider the triangle complex C dual to T, as illustrated in Figure 6.4. Assign one copy of BZ_r to each triangle $t\in C$, and denote it by $\mathrm{BZ}_r^{(v)}$ where v is the inner vertex of T dual to the triangle t. For every edge e adjacent to v, define $\mathrm{pr}_e : \mathrm{BZ}_r^{(v)} \to \mathbb{Z}^r$ to be equal to $\mathrm{pr}_{e^*} : \mathrm{BZ}_r^{(v)} \to \mathbb{Z}^r$ where $e^*\in C$ is the edge dual to e. All projections are taken in the clockwise direction of the corresponding triangle.

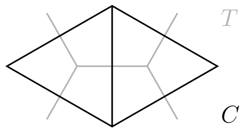


Figure 6.4: Trees and triangle complexes duality

Definition 6.5. Let T be a trivalent graph. We define the affine semigroup of BZ triangles on T as

$$\mathrm{BZ}_{r,T} = \prod_{v \in I} \mathrm{BZ}_r^{(v)} \cap \bigcap_{e=(v_1,v_2), v_1,v_2 \in I} (\mathrm{pr}_e(x^{(v_1)}) = \mathrm{pr}_e^*(x^{(v_2)})).$$

If T is the tripod, then $\mathrm{BZ}_{r,T} = \mathrm{BZ}_r$. Define $\mathrm{pr}_T : BZ_{r,T} \to \mathbb{R}^{3r|I|}$ as the product of $\mathrm{pr} : BZ_r^{(v)} \to \mathbb{R}^{3r}$ with one copy for each $v \in I$.

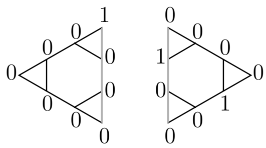


Figure 6.5: BZ triangle on the trivalent 4-leaf tree

Example 6.6. Let T be the trivalent 4-leaf tree and C the triangle complex dual to T as in Figure 6.4. A rank two BZ triangle on T is shown in Figure 6.5.

6.3 Connection Between Group-Based Models and BZ Triangles

For the definition of the polytope $P_{G,T}$ associated with the group-based model with the underlying group G and a tree T, see Definition 1.29.

Lemma 6.7. *Let T be the tripod. Let e_1 be the unique edge directed towards the inner vertex, let e_2 and e_3 be the edges directed away from the inner vertex. The polytope $P_{\mathbb{Z}_{r+1},T}$ has $(r+1)^2$ vertices. They are*

- $x_0^{(e_1)} = x_0^{(e_2)} = x_0^{(e_3)} = 1$ *and all other coordinates zero,*
- $x_0^{(e_1)} = x_i^{(e_2)} = x_{r+1-i}^{(e_3)} = 1$ *for $i \in \{1, \ldots, r\}$ and all other coordinates are zero,*
- $x_i^{(e_1)} = x_i^{(e_2)} = x_0^{(e_3)} = 1$ *for $i \in \{1, \ldots, r\}$ and all other coordinates are zero,*
- $x_i^{(e_1)} = x_0^{(e_2)} = x_i^{(e_3)} = 1$ *for $i \in \{1, \ldots, r\}$ and all other coordinates are zero,*
- $x_i^{(e_1)} = x_j^{(e_2)} = x_k^{(e_3)} = 1$ *for $i, j, k \in \{1, \ldots, r\}$ with $i \equiv j + k \mod (r+1)$ and all other coordinates zero.*

Proof. We can freely choose labels j and k on edges e_2 and e_3, the label $i \equiv j+k \mod (r+1)$ on e_1 is determined by the first two. The additive group $\mathbb{Z}_{r+1}$ has $r+1$ elements, hence there are exactly $(r+1)^2$ possibilities to label the edges of T. Furthermore, x is a vertex of $P_{\mathbb{Z}_{r+1},T}$ if and only if $x_i^{(e_1)} = x_j^{(e_2)} = x_k^{(e_3)} = 1$ with $i \equiv j+k \mod (r+1)$ and all other coordinates are zero. All such possibilities are listed above. $\square$

Let

$$S_{G,T} = \mathbb{N}(P_{G,T} \cap L_{G,T})$$

be the affine semigroup generated by the lattice points of $P_{G,T}$. We will study the connection between $S_{\mathbb{Z}_{r+1},T}$ and $\mathrm{BZ}_{r,T}$.

First, we assume that T is the tripod. The lattice polytope $P_{\mathbb{Z}_{r+1},T}$ and the affine semigroup $S_{\mathbb{Z}_{r+1},T}$ live in the linear subspace of $\mathbb{R}^{3(r+1)}$ defined by $\sum_{h\in G} x_h^{(e)} = 1$ for all edges $e \in E$. Hence, forgetting the coordinate $x_0^{(e)}$ for all $e \in E$ gives a lattice polytope and an affine semigroup isomorphic to $P_{\mathbb{Z}_{r+1},T}$ and $S_{\mathbb{Z}_{r+1},T}$, respectively. We also want to reverse the order of the coordinates corresponding to the edge e_1.

Definition 6.8. Define a linear map $f : \mathbb{R}^{3(r+1)} \to \mathbb{R}^{3r}$ to the vector space of triples of $\mathfrak{g}$-weights by

$$f(x) = (l_1, \ldots, l_r; m_1, \ldots, m_r; n_1, \ldots, n_r)$$

where

$$\begin{aligned} l_i &= x_{r+1-i}^{(e_1)}, \\ m_i &= x_i^{(e_2)}, \\ n_i &= x_i^{(e_3)} \end{aligned}$$

for all $i = 1, \ldots, r$. For every edge e of the tripod, define a linear map $f_e : \mathbb{R}^{r+1} \to \mathbb{R}^r$ by

$$f_e(x) = \begin{cases} (l_1, \ldots, l_r) & \text{if } e = e_1, \\ (m_1, \ldots, m_r) & \text{if } e = e_2, \\ (n_1, \ldots, n_r) & \text{if } e = e_3. \end{cases}$$

Corollary 6.9. *Let T be the tripod. Let e_1 be the unique edge directed towards the inner vertex, let e_2 and e_3 be the edges directed away from the inner vertex. The polytope $f(P_{\mathbb{Z}_{r+1},T})$ has $(r+1)^2$ vertices. They are*

- *the zero vertex,*
- *$m_i = n_{r+1-i} = 1$ for a fixed $i \in \{1, \ldots, r\}$ and all other coordinates zero,*
- *$l_i = m_{r+1-i} = 1$ for a fixed $i \in \{1, \ldots, r\}$ and all other coordinates zero,*
- *$l_i = n_{r+1-i} = 1$ for a fixed $i \in \{1, \ldots, r\}$ and all other coordinates zero,*
- *$l_i = m_j = n_k = 1$ for fixed $i, j, k \in \{1, \ldots, r\}$ with $i + j + k \equiv 0 \mod (r+1)$ and all other coordinates zero.*

Example 6.10. Let T be the tripod. Labelings of the edges of T with elements of $\mathbb{Z}_2$ and $\mathbb{Z}_3$ such that at the inner vertex the sum of labels on the incoming edge equals the sum of labels on the outgoing edges are shown in Figures 6.6 and 6.7. These labelings correspond to the vertices of $P_{\mathbb{Z}_2,T}$ and $P_{\mathbb{Z}_3,T}$. The vertices of $f(P_{\mathbb{Z}_2,T})$ and $f(P_{\mathbb{Z}_3,T})$ without the zero vertex correspond one-to-one with the minimal generators of the semigroup of rank one and rank two BZ triangles as in Example 6.3. We will prove in the next theorem that there is a similar connection between rank r BZ triangles and the group-based model with the underlying group $\mathbb{Z}_{r+1}$.

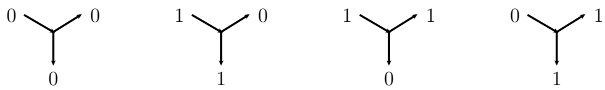


Figure 6.6: Labelings of the tripod with elements of $\mathbb{Z}_2$

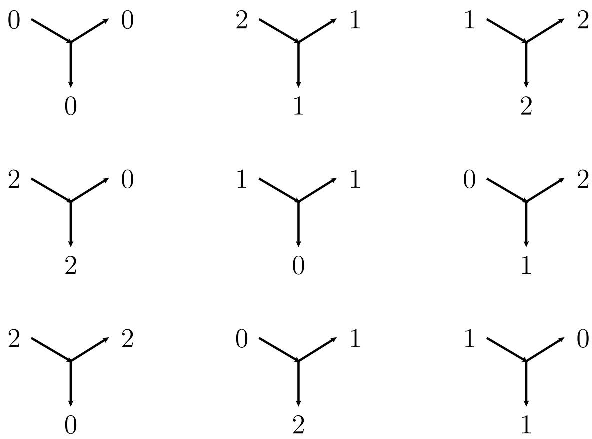


Figure 6.7: Labelings of the tripod with elements of $\mathbb{Z}_3$

Theorem 6.11. *Let T be the tripod. For $r \in \mathbb{N}$,*

$$\mathrm{pr}(\mathrm{BZ}_r) \supseteq f(S_{\mathbb{Z}_{r+1},T}).$$

For $r \in \{1, 2\}$, the inclusion is equality.

Proof. We will prove that every vertex of $f(P_{\mathbb{Z}_{r+1},T})$ is in $\mathrm{pr}(\mathrm{BZ}_r)$. This implies the desired inclusion $f(S_{\mathbb{Z}_{r+1},T}) \subseteq \mathrm{pr}(BZ_r)$, since $S_{\mathbb{Z}_{r+1},T}$ is generated by the vertices of $P_{\mathbb{Z}_{r+1},T}$ and the map f induces an isomorphism between $S_{\mathbb{Z}_{r+1},T}$ and $f(S_{\mathbb{Z}_{r+1},T})$.

- The zero vertex of $f(P_{\mathbb{Z}_{r+1},T})$ equals the projection of the zero BZ triangle.
- Let $i \in \{1, \ldots, r\}$. Define x as follows: $x(0, 2(r-i), 2i-1) = x(2, 2(r-i)-2, 2i-1) = \ldots = x(2(r-i), 0, 2i-1) = 1$ and all other coordinates equal to zero. By condition

(6.1), x is a BZ triangle. The vertex of $f(P_{\mathbb{Z}_{r+1},T})$ with $m_i = n_{r+1-i} = 1$ and all other coordinates zero equals $\mathrm{pr}(x)$.

- Let $i \in \{1, \dots, r\}$. Define x as follows: $x(2(r-i), 2i-1, 0) = x(2(r-i)-2, 2i-1, 2) = \dots = x(0, 2i-1, 2(r-i)) = 1$ and all other coordinates equal to zero. By condition (6.1), x is a BZ triangle. The vertex of $f(P_{\mathbb{Z}_{r+1},T})$ with $l_i = m_{r+1-i} = 1$ and all other coordinates zero equals $\mathrm{pr}(x)$.

- Let $i \in \{1, \dots, r\}$. Define x as follows: $x(2(r-i)+1, 2(i-1), 0) = x(2(r-i)+1, 2(i-1)-2, 2) = \dots = x(2(r-i)+1, 0, 2(i-1)) = 1$ and all other coordinates equal to zero. By condition (6.1), x is a BZ triangle. The vertex of $f(P_{\mathbb{Z}_{r+1},T})$ with $l_i = n_{r+1-i} = 1$ and all other coordinates zero equals $\mathrm{pr}(x)$.

- Let $i, j, k \in \{1, \dots, r\}$ with $i+j+k = r+1$. Note that $2(i+j+k)-3 = 2r+2-3 = 2r-1$. Define x as follows:

$$
\begin{aligned}
&x(2k, 2i-1, 2j-2) = x(2k+2, 2i-1, 2j-4) = \dots = x(2(r-i), 2i-1, 0) = 1,\\
&x(2k-2, 2i, 2j-1) = x(2k-4, 2i+2, 2j-1) = \dots = x(0, 2(r-j), 2j-1) = 1,\\
&x(2k-1, 2i-2, 2j) = x(2k-1, 2i-4, 2j+2) = \dots = x(2k-1, 0, 2(r-j)) = 1
\end{aligned}
$$

  and all other coordinates zero. The vertex of $f(P_{\mathbb{Z}_{r+1},T})$ with $l_i = m_i = n_i = 1$ and all other coordinates zero equals $\mathrm{pr}(x)$.

- Let $i, j, k \in \{1, \dots, r\}$ with $i + j + k = 2(r+1)$. Note that $6r - 2(i+j+k) + 3 = 6r - 4r - 4 + 3 = 2r - 1$. Define x as follows:

$$
\begin{aligned}
&x(2(r-i)+1, 2(r-j)+2, 2(r-k)) = x(2(r-i)+1, 2(r-j)+4, 2(r-k)-2)\\
&\;= \dots = x(2(r-i)+1, 2(i-1), 0) = 1,\\
&x(2(r-i), 2(r-j)+1, 2(r-k)+2) = x(2(r-i)-2, 2(r-j)+1, 2(r-k)+4)\\
&\;= \dots = x(0, 2(r-j)+1, 2(i-1)) = 1,\\
&x(2(r-i)+2, 2(r-j), 2(r-k)+1) = x(2(r-i)+4, 2(r-j)-2, 2(r-k)+1)\\
&\;= \dots = x(2(i-1), 0, 2(r-k)+1) = 1
\end{aligned}
$$

  and all other coordinates zero. The vertex of $f(P_{\mathbb{Z}_{r+1},T})$ with $l_i = m_i = n_i = 1$ and all other coordinates zero equals $\mathrm{pr}(x)$.

Example 6.10 proves the equality for $r \in \{1, 2\}$. □

Remark. Moreover, the semigroups BZ_1 and $f(S_{\mathbb{Z}_2,T})$ are isomorphic. Although we have $\mathrm{pr}(\mathrm{BZ}_2) = f(S_{\mathbb{Z}_3,T})$, the semigroups BZ_2 and $f(S_{\mathbb{Z}_3,T})$ are not isomorphic. The toric ideal corresponding to the semigroup BZ_2 is generated by one cubic polynomial, whereas the toric ideal corresponding to $f(S_{\mathbb{Z}_3,T})$ is generated by two cubic polynomials. For $r \geq 3$, also the inclusion $\mathrm{pr}(\mathrm{BZ}_r) \supseteq f(S_{\mathbb{Z}_{r+1},T})$ is strict. A rank r BZ triangle with the projection $(1,0,\dots,0,1;0,1,0,\dots,0;0,\dots,0,1,0)$ is not in $f(S_{\mathbb{Z}_{r+1},T})$.

Corollary 6.12. *Let T be the tripod. For $r \in \mathbb{N}$, the elements of $S_{\mathbb{Z}_{r+1},T}$ can be labeled by non-trivial triple tensor product invariants.*

Proof. The statement follows from Theorems 6.11 and 6.4. $\square$

Now we state a similar result for any trivalent tree T. Define $f_T : \mathbb{R}^{|E|(r+1)} \to \mathbb{R}^{3r|I|}$ as the direct product of $f : \mathbb{R}^{3(r+1)} \to \mathbb{R}^{3r}$ with one copy for each $v \in I$.

Corollary 6.13. *Let T be a trivalent tree. For $r \in \mathbb{N}$,*

$$\mathrm{pr}_T(\mathrm{BZ}_{r,T}) \supseteq f_T(S_{\mathbb{Z}_{r+1},T}).$$

Furthermore, for $r \in \{1, 2\}$, the equality holds.

Proof. Maps pr_T and f_T are direct products of pr and f with one copy for each $v \in I$. We have

$$\mathrm{pr}_T(\mathrm{BZ}_{r,T}) = \prod_{v \in I} \mathrm{pr}(\mathrm{BZ}_r^{(v)}) \cap \bigcap_{e=(v_1,v_2), v_1,v_2 \in I} (\mathrm{pr}_e(x^{(v_1)}) = \mathrm{pr}_e^*(x^{(v_2)})).$$

We need to show that, for every inner edge $e = (v_1, v_2)$, the map $f_e : S_{\mathbb{Z}_{r+1},T_{v_1}} \to \mathbb{R}^r$ is equal to $f_e : S_{\mathbb{Z}_{r+1},T_{v_2}} \to \mathbb{R}^r$ reversed where T_{v_i} is the tripod with the inner vertex v_i for $i = 1, 2$. Indeed, because in one case e is directed towards the inner vertex and in the other case e is directed away from the inner vertex, then in the first case we have $f_e(x) = (x_r^{(e)}, x_{r-1}^{(e)}, \ldots, x_1^{(e)})$ and in the second case we have $f_e(x) = (x_1^{(e)}, x_2^{(e)}, \ldots, x_r^{(e)})$. $\square$

Remark. Since the inclusion in Theorem 6.11 is strict for $r \geq 3$, also the inclusion in Corollary 6.13 is strict for $r \geq 3$.

In a joint paper with Christopher Manon, further connections between semigroups associated with conformal block algebras and graded semigroups

$$S_{G,T}^{gr} = \mathrm{cone}(P_{G,T} \times \{1\}) \cap (L_{G,T} \times \{1\})$$

will be established.

Appendix A

Program Code: Hilbert Polynomial of the Kimura 3-Parameter Model

```
use application 'polytope';

# Find the number of the lattice points for the 3-leaf tree.
use vars '$s', '$t', '$B', '$m', '$sm', '$ineq';
use vars '$fix', '$i', '$j', '$k', '$l','$eq', '$a';
use vars '$point', '$counter', '@points';

# Define the polytope associated to the Kimura 3-parameter model
# on the 3-leaf tree.
$s=new Polytope<Rational>(POINTS=><<".");
1 1 0 0 0 1 0 0 0 1 0 0 0
1 1 0 0 0 0 1 0 0 0 1 0 0
1 0 1 0 0 1 0 0 0 0 1 0 0
1 0 1 0 0 0 1 0 0 1 0 0 0
1 1 0 0 0 0 0 1 0 0 0 1 0
1 0 0 1 0 1 0 0 0 0 0 1 0
1 0 0 1 0 0 0 1 0 1 0 0 0
1 1 0 0 0 0 0 0 1 0 0 0 1
1 0 0 0 1 1 0 0 0 0 0 0 1
1 0 0 0 1 0 0 0 1 1 0 0 0
1 0 0 1 0 0 1 0 0 0 0 0 1
1 0 0 1 0 0 0 0 1 0 1 0 0
1 0 1 0 0 0 0 0 1 0 0 1 0
1 0 1 0 0 0 0 1 0 0 0 0 1
1 0 0 0 1 0 0 1 0 0 1 0 0
1 0 0 0 1 0 1 0 0 0 0 1 0
.
```

```
# Apply the vertex lattice normalization to $s.
$t=vertex_lattice_normalization($s);
# Basis transformation matrix taking vertices of $s to vertices of $t.
$B=new Matrix<Rational>(<<".");
1 -3 -3 -2 -2 -1 -1 -3 -1 0
0 3/4 3/2 1/2 1 1/4 1/2 3/2 1/2 0
0 3/4 1/2 1/2 1 1/4 1/2 1/2 0 0
0 3/4 1/2 1/2 0 1/4 1/2 1/2 1/2 -1/2
0 3/4 1/2 1/2 0 1/4 -1/2 1/2 0 1/2
0 3/2 3/4 1 1/2 1/2 1/4 0 0 0
0 1/2 3/4 1 1/2 1/2 1/4 1 1/2 0
0 1/2 3/4 0 1/2 1/2 1/4 1 0 1/2
0 1/2 3/4 0 1/2 -1/2 1/4 1 1/2 -1/2
0 3/4 3/4 1/2 1/2 1/4 1/4 3/2 1/2 0
0 3/4 3/4 1/2 1/2 1/4 1/4 1/2 0 0
0 3/4 3/4 1/2 1/2 1/4 1/4 1/2 1/2 -1/2
0 3/4 3/4 1/2 1/2 1/4 1/4 1/2 0 1/2
.

# Matrix $m for multiplying the vertices of $s by 3.
$m=new Matrix<Rational>(<<".");
1 0 0 0 0 0 0 0 0 0 0 0 0
0 3 0 0 0 0 0 0 0 0 0 0 0
0 0 3 0 0 0 0 0 0 0 0 0 0
0 0 0 3 0 0 0 0 0 0 0 0 0
0 0 0 0 3 0 0 0 0 0 0 0 0
0 0 0 0 0 3 0 0 0 0 0 0 0
0 0 0 0 0 0 3 0 0 0 0 0 0
0 0 0 0 0 0 0 3 0 0 0 0 0
0 0 0 0 0 0 0 0 3 0 0 0 0
0 0 0 0 0 0 0 0 0 3 0 0 0
0 0 0 0 0 0 0 0 0 0 3 0 0
0 0 0 0 0 0 0 0 0 0 0 3 0
0 0 0 0 0 0 0 0 0 0 0 0 3
.
# Define the polytope $sm as the convex hull of the vertices of $s
# multiplied by 3.
$sm=new Polytope<Rational>(VERTICES=>($s->VERTICES)*$m);
# $ineq contains facet inequalities for $sm.
$ineq=($sm->FACETS);

# Loop that finds the number of the lattice points for the polytope
```

```
# 3*$s with the first 4 coordinates fixed.
$counter=0;
# The 2nd to 5th coordinate of $sm can take integer values
# from 0 to 3, which sum up to 3.
for $i (0...3){
for $j (0...(3-$i)){
for $k (0...(3-$i-$j)){
$l=3-$i-$j-$k;
# Matrix $fix for equalities that fix 2nd to 5th coordinate.
$fix=new Matrix<Rational>(<<".");
-$i 1 0 0 0 0 0 0 0 0 0 0 0
-$j 0 1 0 0 0 0 0 0 0 0 0 0
-$k 0 0 1 0 0 0 0 0 0 0 0 0
-$l 0 0 0 1 0 0 0 0 0 0 0 0
.

# Define a new set of equalities by taking the affine hull of $sm and $fix.
$eq=($sm->AFFINE_HULL)/$fix;
# Define a new polytope $a using the new set of equalities $eq and the
# inequalities of $sm.
$a=new Polytope<Rational>(INEQUALITIES=>$ineq,EQUATIONS=>$eq);
# Apply the basis transformation matrix to $a and count the lattice points.
$a=new Polytope<Rational>(POINTS=>($a->VERTICES)*$B);
$point=($a->N_LATTICE_POINTS);
# Remember all the results in the array $points.
$points[$counter]=$point;
$counter++;
}
}
}


#Find the number of the lattice points for 4-leaf tree.
use vars '$p', '$r', '$A', '$m', '$pm', '$ineq';
use vars '$i', '$j', '$k', '$l', '$w', '$x', '$y', '$z';
use vars '$e', '$f', '$g', '$h';
use vars '$fix', '$eq', '$a', '$point', '$sum1', '$sum2';
use vars '$counter1', '$counter2', '@points1', '@points2';

# Define the polytope of the Kimura 3-parameter model on the 4-leaf tree.
$p=new Polytope<Rational>(POINTS=><<".");
1 1 0 0 0 1 0 0 0 1 0 0 0 1 0 0 0 1 0 0 0
```

```
1 1 0 0 0 1 0 0 0 1 0 0 0 0 0 1 0 0 0 1 0
1 1 0 0 0 1 0 0 0 1 0 0 0 0 1 0 0 0 1 0 0
1 1 0 0 0 1 0 0 0 1 0 0 0 0 0 0 1 0 0 0 1
1 1 0 0 0 0 0 1 0 0 0 1 0 1 0 0 0 0 0 1 0
1 1 0 0 0 0 0 1 0 0 0 1 0 0 0 1 0 1 0 0 0
1 1 0 0 0 0 0 1 0 0 0 1 0 0 1 0 0 0 0 0 1
1 1 0 0 0 0 0 1 0 0 0 1 0 0 0 0 1 0 1 0 0
1 1 0 0 0 0 1 0 0 0 1 0 0 1 0 0 0 0 1 0 0
1 1 0 0 0 0 1 0 0 0 1 0 0 0 0 1 0 0 0 0 1
1 1 0 0 0 0 1 0 0 0 1 0 0 0 1 0 0 1 0 0 0
1 1 0 0 0 0 1 0 0 0 1 0 0 0 0 0 1 0 0 1 0
1 1 0 0 0 0 0 0 1 0 0 0 1 1 0 0 0 0 0 0 1
1 1 0 0 0 0 0 0 1 0 0 0 1 0 0 1 0 0 1 0 0
1 1 0 0 0 0 0 0 1 0 0 0 1 0 1 0 0 0 0 1 0
1 1 0 0 0 0 0 0 1 0 0 0 1 0 0 0 1 1 0 0 0
1 0 0 1 0 1 0 0 0 0 0 1 0 1 0 0 0 0 0 1 0
1 0 0 1 0 1 0 0 0 0 0 1 0 0 0 1 0 1 0 0 0
1 0 0 1 0 1 0 0 0 0 0 1 0 0 1 0 0 0 0 0 1
1 0 0 1 0 1 0 0 0 0 0 1 0 0 0 0 1 0 1 0 0
1 0 0 1 0 0 0 1 0 1 0 0 0 1 0 0 0 1 0 0 0
1 0 0 1 0 0 0 1 0 1 0 0 0 0 0 1 0 0 0 1 0
1 0 0 1 0 0 0 1 0 1 0 0 0 0 1 0 0 0 1 0 0
1 0 0 1 0 0 0 1 0 1 0 0 0 0 0 0 1 0 0 0 1
1 0 0 1 0 0 1 0 0 0 0 0 1 1 0 0 0 0 0 0 1
1 0 0 1 0 0 1 0 0 0 0 0 1 0 0 1 0 0 1 0 0
1 0 0 1 0 0 1 0 0 0 0 0 1 0 1 0 0 0 0 1 0
1 0 0 1 0 0 1 0 0 0 0 0 1 0 0 0 1 1 0 0 0
1 0 0 1 0 0 0 0 1 0 1 0 0 1 0 0 0 0 1 0 0
1 0 0 1 0 0 0 0 1 0 1 0 0 0 0 1 0 0 0 0 1
1 0 0 1 0 0 0 0 1 0 1 0 0 0 1 0 0 1 0 0 0
1 0 0 1 0 0 0 0 1 0 1 0 0 0 0 0 1 0 0 1 0
1 0 1 0 0 1 0 0 0 0 1 0 0 1 0 0 0 0 1 0 0
1 0 1 0 0 1 0 0 0 0 1 0 0 0 0 1 0 0 0 0 1
1 0 1 0 0 1 0 0 0 0 1 0 0 0 1 0 0 1 0 0 0
1 0 1 0 0 1 0 0 0 0 1 0 0 0 0 0 1 0 0 1 0
1 0 1 0 0 0 0 1 0 0 0 0 1 1 0 0 0 0 0 0 1
1 0 1 0 0 0 0 1 0 0 0 0 1 0 0 1 0 0 1 0 0
1 0 1 0 0 0 0 1 0 0 0 0 1 0 1 0 0 0 0 1 0
1 0 1 0 0 0 0 1 0 0 0 0 1 0 0 0 1 1 0 0 0
1 0 1 0 0 0 1 0 0 1 0 0 0 1 0 0 0 1 0 0 0
1 0 1 0 0 0 1 0 0 1 0 0 0 0 0 1 0 0 0 1 0
1 0 1 0 0 0 1 0 0 1 0 0 0 0 1 0 0 0 1 0 0
```

```
1 0 1 0 0 0 1 0 0 1 0 0 0 0 0 0 1 0 0 0 1
1 0 1 0 0 0 0 0 1 0 0 1 0 1 0 0 0 0 0 1 0
1 0 1 0 0 0 0 0 1 0 0 1 0 0 0 1 0 1 0 0 0
1 0 1 0 0 0 0 0 1 0 0 1 0 0 1 0 0 0 0 0 1
1 0 1 0 0 0 0 0 1 0 0 1 0 0 0 0 1 0 1 0 0
1 0 0 0 1 1 0 0 0 0 0 0 1 1 0 0 0 0 0 0 1
1 0 0 0 1 1 0 0 0 0 0 0 1 0 0 1 0 0 1 0 0
1 0 0 0 1 1 0 0 0 0 0 0 1 0 1 0 0 0 0 1 0
1 0 0 0 1 1 0 0 0 0 0 0 1 0 0 0 1 1 0 0 0
1 0 0 0 1 0 0 1 0 0 1 0 0 1 0 0 0 0 1 0 0
1 0 0 0 1 0 0 1 0 0 1 0 0 0 0 1 0 0 0 0 1
1 0 0 0 1 0 0 1 0 0 1 0 0 0 1 0 0 1 0 0 0
1 0 0 0 1 0 0 1 0 0 1 0 0 0 0 0 1 0 0 1 0
1 0 0 0 1 0 1 0 0 0 0 1 0 1 0 0 0 0 0 1 0
1 0 0 0 1 0 1 0 0 0 0 1 0 0 0 1 0 1 0 0 0
1 0 0 0 1 0 1 0 0 0 0 1 0 0 1 0 0 0 0 0 1
1 0 0 0 1 0 1 0 0 0 0 1 0 0 0 0 1 0 1 0 0
1 0 0 0 1 0 0 0 1 1 0 0 0 1 0 0 0 1 0 0 0
1 0 0 0 1 0 0 0 1 1 0 0 0 0 0 1 0 0 0 1 0
1 0 0 0 1 0 0 0 1 1 0 0 0 0 1 0 0 0 1 0 0
1 0 0 0 1 0 0 0 1 1 0 0 0 0 0 0 1 0 0 0 1
.
# Apply vertex lattice normalization to $p.
$r=vertex_lattice_normalization($p);
# Basis transformation matrix taking vertices of $p to vertices of $r.
$A=new Matrix<Rational>(<<".");
1 3 -1 0 3 1 -1 1 3 -3 -1 1 -1 -1 -1 -2
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 0 0 0 0 0 0 0 1/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -1 1 1 0 0 0 1/2 3/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -1 1 0 0 1/2 1/2 0 1/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -1 1 0 -1 1/2 1/2 1/2 3/4
0 -3/4 1/4 0 0 -1/4 0 0 -3/4 0 1/4 -1/4 0 0 0 1/4
0 -3/4 1/4 0 -1 -1/4 1 0 -3/4 1 1/4 -1/4 0 0 1/2 3/4
0 -3/4 1/4 0 -1 -1/4 0 0 -3/4 1 1/4 -1/4 1/2 1/2 0 1/4
0 -3/4 1/4 0 -1 -1/4 0 -1 -3/4 1 1/4 -1/4 1/2 1/2 1/2 3/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -3/4 3/2 1/4 -1/4 1/2 1/4 1/2 1/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -3/4 1/2 1/4 -1/4 1/2 1/4 0 1/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -3/4 1/2 1/4 -1/4 0 1/4 1/2 3/4
0 -3/4 1/4 0 -3/4 -1/4 1/4 -1/4 -3/4 1/2 1/4 -1/4 0 1/4 0 3/4
0 0 0 -3/4 -3/4 0 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 1/4 1/4 1/4
0 -1 1 1/4 -3/4 0 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 1/4 1/4 3/4
0 -1 0 1/4 -3/4 0 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 3/4 1/4 3/4
```

```
0 -1 0 1/4 -3/4 -1 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 -1/4 1/4 1/4
0 -3/4 1/4 3/4 -3/4 -1/4 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 1/2 1/4 1
0 -3/4 1/4 -1/4 -3/4 -1/4 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 1/2 1/4 1/2
0 -3/4 1/4 -1/4 -3/4 -1/4 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 0 1/4 1/2
0 -3/4 1/4 -1/4 -3/4 -1/4 1/4 -1/4 -3/4 3/4 1/4 -1/4 1/4 0 1/4 0
.

# Matrix $m for multiplying the vertices of $p by 3.
$m=new Matrix<Rational>(<<".");
1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
.
# Define the polytope $pm as the convex hull of the vertices of $p
# multiplied by 3.
$pm=new Polytope<Rational>(VERTICES=>($p->VERTICES)*$m);
# $ineq contains facet inequalities for $pm.
$ineq=($pm->FACETS);

# Loop that finds the number of the lattice points for the polytope
# 3*$p with 14th to 21th coordinate fixed (corresponding to 2
# incident leaf edges) and with 14th to 17th coordinate fixed
# (corresponding to 1 leaf edge).
$counter1=0;
```

```
# The 14th to 21th coordinate of 3*$s can take integer values
# from 0 to 3, coordinates 14 to 17 sum up to 3 and
# coordinates 18 to 21 sum up to 3.
for $i (0...3){
for $j (0...(3-$i)){
for $k (0...(3-$i-$j)){
$sum1=0;
$counter2=0;
for $w (0...3){
for $x (0...(3-$w)){
for $y (0...(3-$w-$x)){
# Loop that fixes 2nd to 5th coordinate corresponding to an
# additional leaf edge to make computations faster. We find
# the number of the lattice points separately for each possible
# integer fixation and then sum over all the values.
$sum2=0;
for $e (0...3){
for $f (0...(3-$e)){
for $g (0...(3-$e-$f)){
$l=3-$i-$j-$k;
$z=3-$w-$x-$y;
$h=3-$e-$f-$g;
# Matrix for equalities that fix coordinates under
# consideration.
$fix=new Matrix<Rational>(<<".");
-$i 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0
-$j 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0
-$k 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0
-$l 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0
-$w 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0
-$x 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0
-$y 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0
-$z 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-$e 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-$f 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-$g 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-$h 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
.
# Define a new set of equalities by taking the affine hull of
# $pm and $fix.
$eq=($pm->AFFINE_HULL)/$fix;
# Define a new polytope $a using the new set of equalities $eq and
```

```
# the inequalities of $pm.
$a=new Polytope<Rational>(INEQUALITIES=>$ineq,EQUATIONS=>$eq);
# Apply the basis transformation matrix to $a and count
# the lattice points.
$a=new Polytope<Rational>(POINTS=>($a->VERTICES)*$A);
$point=$a->N_LATTICE_POINTS;
# Sum the number of the lattice points over all possible integer
# values corresponding to the additional leaf edge.
$sum2=$sum2+$point;
}
}
}
# Array @points2 holds the number of the lattice points when 14th
# to 21st coordinate are fixed.
$points2[($counter1*20)+$counter2]=$sum2;
$sum1=$sum1+$sum2;
$counter2++;
}
}
}
# Array @points1 holds the number of the lattice points when 14th
# to 17th coordinate are fixed.
$points1[$counter1]=$sum1;
$counter1++;
}
}
}

use vars '$sum';

# Finding the total number of the lattice points by using the
# formulas (there are 20 possibilities for integer values
# corresponding to one edge).
$sum=0;
for $i(0...19){
for $j(0...19){
$sum=$sum+($points2[($i*20)+$j]*$points[$i]*$points[$j]);
}
}
print "Snowflake has $sum lattice points. \n \n";

$sum=0;
```

```
for $i(0...19){
$sum=$sum+($points1[$i]*$points1[$i]);
}
print "3-caterpillar has $sum lattice points. \n";
```

Anhang B

Zusammenfassung

Phylogenetische algebraische Geometrie beschäftigt sich mit algebraischen Varietäten die mit phylogenetischen Modellen assoziiert sind. In dieser Dissertation werden Gitterpolytope und affine Halbgruppen untersucht, die mit torischen Varietäten von gruppenbasierten phylogenetischen Modellen korrespondieren.

Laut einem Resultat von Buczyńska und Wiśniewski ist die Hilbertfunktion der algebraischen Varietät auf dem Jukes-Cantor binären Modell und einem trivalenten Baum unabhängig von der Topologie des Baumes [BW07]. In Zusammenarbeit mit Haase und Paffenholz geben wir einen einfachen kombinatorischen Beweis für diesen Satz. Außerdem zeigen wir, dass die analoge Aussage für das Kimura Dreiparametermodell nicht stimmt [Kub12].

Buczyńska und Wiśniewski haben auch gezeigt, dass die mit dem Jukes-Cantor binären Modell assoziierte Halbgruppe im Grad eins erzeugt ist [BW07]. Eine phylogenetische Halbgruppe auf einem Graph verallgemeinert das Jukes-Cantor binäre Modell auf einem Baum [Buc12, BBKM11]. Wir zeigen, dass es für jede natürliche Zahl g einen Graph gibt, sodass der maximale Grad vom minimalen Erzeugendensystem von der entsprechenden phylogenetischen Halbgruppe genau $2\lfloor \frac{g}{2} \rfloor + 1$ ist. Das ist Teil der Arbeit mit Buczyńska, Buczyński und Michałek [BBKM11], in der wir auch zeigen, dass $g + 1$ die bestmögliche obere Schranke ist.

Das minimale Erzeugendensystem der phylogenetischen Halbgruppe auf einem trivalenten Baum wurde von Buczyńska und Wiśniewski untersucht [BW07] und der Fall von trivalenten Graphen mit erster Bettizahl eins wurde von Buczyńska betrachtet [Buc12]. Wir beschreiben das minimale Erzeugendensystem auf allen Graphen mit erster Bettizahl $g \leq 1$ und auf allen trivalenten Graphen mit erster Bettizahl zwei. Außerdem beschreiben wir für beliebige trivalente Graphen die minimalen Erzeuger vom Grad $d \leq 2$.

Basierend auf der Arbeit von Sturmfels und Xu [SX10] hat Manon gezeigt, dass die phylogenetischen Halbgruppen torische Degenerationen von Algebren $\mathrm{SL}_2(\mathbb{C})$-konformer Blöcke sind [Man09]. Darüber hinaus hat er ähnliche Verbindungen zwischen dem Rang zweier Berenstein-Zelevinsky-Dreiecke und Algebren $\mathrm{SL}_3(\mathbb{C})$-konformer Blöcke gezeigt [Man12a]. Motiviert von diesen Resultaten stellen wir eine Verbindung zwischen affinen Halbgruppen von gruppenbasierten Modellen und Halbgruppen von Berenstein-Zelevinsky-Dreiecken her.

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