PHYLOGENETIC TORIC VARIETIES ON GRAPHS

A Dissertation

by

WERONIKA JULIA BUCZYŃSKA

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

August 2010

Major Subject: Mathematics

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Approved by:

Chair of Committee,	Frank Sottile
Committee Members,	Gabriel Dos-Reis
	Paulo Lima-Filho
	Laura Felicia Matusevich
Head of Department,	Al Boggess

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ABSTRACT

Phylogenetic Toric Varieties on Graphs. (August 2010)

Weronika Julia Buczyńska, B.S, Warsaw University;

M.S., Warsaw University

Chair of Advisory Committee: Dr. Frank Sottile

We define the phylogenetic model of a trivalent graph as a generalization of a binary symmetric model of a trivalent phylogenetic tree. If the underlining graph is a tree, the model has a parametrization that can be expressed in terms of the tree. The model is always a polarized projective toric variety. Equivalently, it is a projective spectrum of a semigroup ring. We describe explicitly the generators of this projective coordinate ring for graphs with at most one cycle. We prove that models of graphs with the same topological invariants are deformation equivalent and share the same Hilbert function. We also provide an algorithm to compute the Hilbert function, which uses the structure of the graph as a sum of elementary ones. Also, this Hilbert function of phylogenetic model of a graph with g cycles is meaningful for the theory of connections on a Riemann surface of genus g.

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CHAPTER I

INTRODUCTION AND BACKGROUND

The inspiration for this work are toric varieties arising in computational biology, or more precisely in phylogenetic algebraic geometry. The references to the subject include [8], [19] and [21].

Markov models on phylogenetic trees are statistical models describing evolution. They are usually defined as a subset of the probability simplex, parametrized by a subset of matrices depending on the model. Among them there are group-based models on phylogenetic trees. These are special, as their projective versions, that is the Zariski closure of the parametrization in the complex projective space, are projective toric varieties.

In this thesis we are interested in the simplest group-based models — binary symmetric models, also called the Jukes-Cantor models, on trivalent trees. The object of study in this thesis is the generalization of those models to trivalent graphs.

The thesis is organized in the following way: further in this chapter, in Section I.1, we give motivation to the subject and point out references where the main object of our study appears. Then we give a brief introduction to our main tools: we recall geometric invariant theory in Section I.3, next, in Section I.4, we set the notation for projective toric varieties and provide the description of GIT quotient of a projective toric variety by subtorus of its big torus.

In Section II.1 we state combinatorial relations between the topological invariants of a trivalent graph and we prove that graphs with the same invariants are mutation-equivalent. Next, in Section II.2 we review the parametric description of the tree

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The journal model is Journal of the American Mathematical Society.

models from [4]. In Section II3 we define the model of a trivalent graph as a GIT quotient of a product of $\mathbb{P}^3$'s indexed by inner vertices of the graph. This implies that the model is toric and comes with an embedding into a weighted projective space. Our first result is Theorem II.37 that lists the set of minimal generators of the projective coordinate ring of the model, when the underlying graph has the first Betti number at most one. Chapter III contains our second result — models of mutation-equivalent graphs are deformation equivalent.

Theorem III.5. *Geometric models of connected trivalent graphs with n leaves and the first Betti number g are deformation equivalent in the projective toric variety $\mathbb{P}_{g,n}$, which is a quotient of $\mathbb{P}^{2^{n+2g-1}-1}$ by a g-dimensional torus.*

In Chapter IV we prove that the Hilbert functions of mutation-equivalent models are equal (Theorem IV.5) and finally we compute these Hilbert functions explicitly.

1. Motivation — Markov models on phylogenetic trees

A *phylogenetic tree* is an acyclic connected graph with additional data attached to its edges and vertices. At a vertex v there is a finite ordered set A_v called an alphabet. At an edge with ends v and w there is a doubly-stochastic matrix (all rows and columns sums are 1) with the $(i,j)^{th}$ entry indicating the probability of the i^{th} letter of A_v being changed to the j^{th} letter A_w. To construct a *Markov model* on a phylogenetic tree we first need to indicate a set of observable vertices, for example the leaves of the tree. Then the model is the subvariety of the probability simplex, parametrized by a subset of matrices that we only allow, given by probabilities of observing letters at the observable vertices. We consider symmetric models, which means we allow symmetric matrices. Typically the observable vertices are the leaves of the tree.

Apart form this real variety, one can consider its complex algebraic relaxation.

That is, the parameters are allowed to vary in a complex projective space and we take the Zariski closure of the image. Then the model becomes a complex projective variety and can be studied by means of algebraic geometry. Binary symmetric models have additional structure — they are equipped with an action of a torus of dimension equal to the dimension of the model and thus they are projective toric varieties. This is an especially nice class of varieties, which have a combinatorial description by lattice polytopes. The geometry of the simplest group-based models — binary symmetric models with the restriction that the underlying tree is trivalent was the object of study of [5]. In that paper we described the corresponding lattice polytope and interpreted the models as a certain quotient of a product of three-dimensional projective spaces.

2. Toric algebras of our graph models in the literature

We generalize the quotient description of the tree models introduced in [5] and we again have a toric projective model, which this time is embedded in a weighted projective space. Such an embedding is always given by a graded lattice cone. We denote the cone for a graph $\mathcal{G}$ by $\tau(\mathcal{G})$.

The way we associate a lattice cone to a trivalent graph appears also in the work of Manon [15]. He constructs a sheaf of algebras over the moduli stack $\mathcal{M}_{g,n}$ of genus g curves with n marked points and our semigroup algebras $\mathbb{C}[\tau(\mathcal{G})]$ are obtained by some initial term deformations from algebras above the most special points of $\mathcal{M}_{g,n}$ in Manon's construction.

Another place where our cones $\tau(\mathcal{G})$ appear is the Jeffrey and Weitsmann's [14] study of flat $SU(2)$-connections on a genus g Riemann surface. In their context the trivalent graph $\mathcal{G}$ describes the geometry of the compact surface Σ^g of genus g and

thus has no leaves. A subset of $\mathbb{Z}$-labellings of the graph, which are exactly points of our cone $\tau(\mathcal{G})$, are in 1–1 correspondence with the number of Bohr-Sommerfeld fibers which is the central object of study in [14]. By the Verlinde formula, the number of those fibers equals the dimension of holomorphic sections of powers of a natural line bundle on the moduli space of flat $SU(2)$ connections on Σ^g. This number is a value of the Hilbert function of the toric model of a connected graph with no leaves and the first Betti number g.

By Theorem IV.5, we know that the Hilbert function only depends on the topological invariants of the graph.

Although the model depends on the shape of the underlying trivalent tree, once we restrict ourselves to trees with fixed number of leaves, models of all of them are in the same irreducible component of the Hilbert scheme of projective varieties with fixed Hilbert polynomial. This was proved by Sturmfels and Xu in [25].

Any trivalent graph is made by gluing together tripods, that is graphs $\curlyvee$ with four vertices and three edges attached to the central vertex. To construct the toric model we assign to every inner vertex a copy of a three-dimensional complex projective space and to every edge we assign an action of the one-dimensional complex torus $\mathbb{C}^*$ on the product of all those $\mathbb{P}^3$, which corresponds to gluing two tripods along that edge. The model $X(\mathcal{G})$ of the trivalent graph $\mathcal{G}$ is a geometric invariant theory (GIT) quotient of product of the $\mathbb{P}^3$ by the torus defined as a product of the $\mathbb{C}^*$'s corresponding to the internal edges. We also translate this description into language of projective toric varieties, by writing the model $X(\mathcal{G})$ as the projective spectrum of a semigroup ring $\mathbb{C}[\tau(\mathcal{G})]$. The underlying semigroup $\tau(\mathcal{G})$ has a clear description in terms of the graph $\mathcal{G}$.

Three results of this thesis generalize our earlier results obtained in [5] about binary symmetric models of trivalent trees to phylogenetic graph models. First we

describe the minimal $\mathbb{Z}$-generators of the semigroup $\tau(\mathcal{G})$ when the graph $\mathcal{G}$ has the first Betti number at most one. We also prove that models of graphs with the same discrete invariants are deformation equivalent and lastly that they share the same Hilbert function.

3. Geometric invariant theory

Given an algebraic variety X with an action of an algebraic group G, one hopes to construct an algebraic quotient. The naive way to do it, that is to simply take the orbit space, most often leads to a space with non-closed points (not a T1-space. The main tool to construct a quotient which is an algebraic variety with desired properties is geometric invariant theory created by David Mumford in 1960's. His main purpose was to answer questions in the theory of moduli — those are varieties or schemes parametrizing all objects with given invariants. The classical reference to the subject is Mumford's book [17]. This theory assumes that the algebraic group G that acts on X is reductive and the action has a *linearization* with respect to some line bundle on X. Depending on the line bundle the set of (semi-)stable points is determined. There are several types of quotients that one may want to consider. One is the *good geometric quotient*, which is the orbit space of the stable points. The problem with it is that often there are not enough stable points. The good quotient is the *semi-geometric* and *affine* quotient on the set of semi-stable points. From now on we talk about the good quotient.

The resulting quotient is projective if the initial space was projective. The first, most common, example of a GIT quotient is the projective space which is the quotient of $\mathbb{C}^n$ by the action of $\mathbb{C}^*$ — in this case the non-stable locus is the point 0. Toric varieties can be seen as a generalization of the projective space as they are quotients

of open subsets of an affine space.

We use geometric invariant theory for a normal projective variety X with an action of an algebraic torus $\mathbb{T}$. Our main reference is Section 5 and 6 of [2], although the setup we use may seem to be slightly more general then the one found in [2]. This is because instead of linearizing only with respect to a line bundle we allow ample Weil divisors. We will explain the necessary modifications and show how this does not affect the basic theory.

We work on a normal algebraic variety X. We recall some standard notions in algebraic geometry. A **Weil divisor** $\mathcal{L} = \sum n_i D_i$ is a formal sum of codimension one subvarieties D_i of X with integer coefficients. Given a rational function f on X the **principal divisor of** f is the formal difference between the zero locus of f and locus of poles of f (equivalently zeros of $\frac{1}{f}$), both counted with multiplicities. A Weil divisor is called **Cartier** if it is locally principal divisor, which means there is an open covering $\{U_i\}$ of X together with rational functions f_i such that $\mathcal{L} \cap U_i$ is the principal divisor of f_i on U_i. It is standard to identify a Cartier divisor with a line bundle using the cocycle of $\frac{f_i}{f_j}$ on $U_i \cap U_j$, see [13, p.141].

Definition I.1. A divisor $\mathcal{L}$ is an **ample Weil divisor** if some positive multiple $n\mathcal{L}$ is an ample line bundle.

A line bundle is ample if some multiple $m\mathcal{L}$ (equivalently tensor power) of it is very ample. This means that the map defined by the linear system $|m\mathcal{L}|$ is an embedding into a projective space.

Given an ample Weil divisor $\mathcal{L}$ we have the ring

$$R(X, \mathcal{L}) := \bigoplus_{p=0}^{\infty} H^0(X, \mathcal{O}(p\mathcal{L})),$$

which is the projective coordinate ring of X embedded into a weighted projective space

by the linear system $|\mathcal{L}|$. This is completely analogous, see [20], to the standard way of describing embedding of X into a projective space in when $\mathcal{L}$ is a very ample line bundle, see [13, Section II.2]. We discuss those facts in 4.1.

We denote by

$$R_p(X, \mathcal{L}) := R(X, p\mathcal{L})$$

the ring given by a multiple of $\mathcal{L}$. When the divisor $\mathcal{L}$ is clear, we write $R(X)$ and $R_p(X)$ an instead of $R(X, \mathcal{L})$ and $R(X, p\mathcal{L})$.

Lemma I.2 (Veronese embedding)**.** *Let $X = \operatorname{Proj} R(X, \mathcal{L})$ be a projective variety with a distinguished ample Weil divisor $\mathcal{L}$. Then for any positive integer p the inclusion $R_p(X, \mathcal{L}) \hookrightarrow R(X, \mathcal{L})$ induces an isomorphism*

$$\operatorname{Proj} R(X, \mathcal{L}) \simeq \operatorname{Proj} R_p(X, \mathcal{L})$$

Proof. See [10, Chapter 2, Theorem 2.4.7], and also [13, Ex. II 5.13]. □

We briefly recall the definitions of quotients simplifying the statements from [2]. Let G be a reductive algebraic group acting on a variety X. A G-equivariant morphism $\pi : X \to Y$ is called a **semi-geometric quotient** if

- the image of every closed orbit is closed, and this property is invariant under base change
- π is surjective and images of disjoint, closed orbits are disjoint and this property is invariant under base change
- $\pi_*(\mathcal{O}_X^G) = \mathcal{O}_Y$.

The map $\pi : X \to Y$ is called a **good quotient** if it is both affine and semi-geometric. A map $\pi : X \to Y$ is affine if preimage of any affine subset of Y is affine.

This definition implies that the good quotient is a categorical quotient, and thus unique [2, Rmk.3.1 and Thm 3.2].

To construct the quotient, we need some more definitions.

Definition I.3. Let G be a reductive algebraic group acting on X. An ample Weil divisor $\mathcal{L}$ on X is **G-linearized** if the action of G can be lifted to the projective coordinate ring $R(X, \mathcal{L})$. More precisely, the action of G on $X = \operatorname{Proj} R(X, \mathcal{L})$ induced by the lift, is the action of G on X.

When $\mathcal{L}$ is a line bundle, a G-linearization is an action of G on $\mathcal{L}$ which is linear on fibers and agrees with its action on X. We recall the definition of a $\mathcal{L}$-semistable point [2, § 6.1], which is independent of the multiple of $\mathcal{L}$.

Definition I.4. Let $\mathcal{L}$ be an ample Weil divisor. A point $x \in X$ is **$\mathcal{L}$-semistable** if there exists a G-invariant section of a positive multiple of $\mathcal{L}$ that does not vanish at x. We denote by X^{ss} the set of all semistable points. The **GIT quotient** of X by G with respect to the linearization $\mathcal{L}$ is

$$X/\!\!/G = X^{ss}/\!\!/G,$$

where $X^{ss}/\!\!/G$ denotes the good quotient of the set of semistable points with respect to $\mathcal{L}$ by the action of G. The rational map $X \to X/\!\!/G$ is called GIT quotient map and the regular map $X^{ss} \to X/\!\!/G$ is a good quotient map.

Remark I.5. Both [17] and [2] assume that the section in the above definition has an affine support, but as we consider only ample $\mathcal{L}$ all its sections automatically have affine support.

The following theorem says that in the above situation a GIT quotient exists and is the projective spectrum of the ring of invariants.

Theorem I.6. *Let G be a reductive group acting on projective varieties X and Y.*

(i) Let $\mathcal{L}$ be a G-linearized ample Weil divisor on X. Then

$$X/\!\!/G = \operatorname{Proj} R(X, \mathcal{L})^G.$$

(ii) Let $X \hookrightarrow Y$ be a G-equivariant embedding, with $Y = \operatorname{Proj} R$ and $X = \operatorname{Proj} R/I$, where I is the homogeneous ideal of X in Y. Then I is generated by invariants $f_1, \ldots, f_j$, the map $X/\!\!/G \hookrightarrow Y/\!\!/G$ is an embedding and the homogeneous ideal of $X/\!\!/G$ in R^G is also generated by $f_1, \ldots, f_j$.

Proof. In [2, §5] the affine quotient is defined for an affine variety X as a spectrum of invariants and [2, Thm 5.4] says it is a good quotient. Then in [2, §7] there is a characterization of a good quotient $\pi : X \to Y$ as a locally affine quotient, that is the map π is a good quotient if and only if for any open affine subset $U \subset Y$ the restriction of the map π to $\pi^{-1}(U)$ is an affine quotient.

We know from [2, Thm 6.2.1] that (i) is true for projective space and $\mathcal{L} = \mathcal{O}(1)$. Additionally for an arbitrary variety $X = \operatorname{Proj} R$ and a very ample line bundle $\mathcal{L}$ that defines an equivariant embedding into $\mathbb{P}^n$ by [2, §6.3] we have:

- $X^{ss} = (\mathbb{P}^n)^{ss} \cap X$
- the restriction of the good quotient morphism $\pi\colon (\mathbb{P}^n)^{ss} \to (\mathbb{P}^n)^{ss}/\!\!/G$ is the good quotient morphism on X.

We choose an affine covering $\mathcal{U}$ of the quotient $\mathbb{P}^n/\!\!/G$ by sets of the form $\{f \neq 0\}$, where f is G-invariant. Then $\{\pi^{-1}(U) | U \in \mathcal{U}\}$ is an affine G-invariant covering of $\mathbb{P}^n$, since π is an affine map. By [2, Thm 5.3] and the Hilbert-Nagata theorem [2, Thm 5.2] for each $U \in \mathcal{U}$ we know that $(\pi^{-1}(U) \cap X)/\!\!/G$ is a spectrum of invariants

$$(\pi^{-1}(U) \cap X)/\!\!/G = \operatorname{Spec}(R[f^{-1}]^0)^G$$

Also each $\pi^{-1}(U) \cap X$ has form $\{g = \pi^* f|_X \neq 0\}$. To see that $X/\!\!/G = \operatorname{Proj} R^G$, we only need to see that $\left(R^G[g^{-1}]\right)^0 = (R[g^{-1}]^0)^G$, which is true since g is G-invariant. Thus (i) holds for X projective and $\mathcal{L}$ very ample.

When $\mathcal{L}$ is an ample Weil divisor, we use Lemma I.2 to replace $\mathcal{L}$ by its k^{th} power. More precisely, we choose k such that $k\mathcal{L}$ is a very ample line bundle, and since the set of semistable points does not depend on the multiple of $\mathcal{L}$ we have

$$X/\!\!/G = \operatorname{Proj} R_p(X, \mathcal{L})^G = \operatorname{Proj}(R(X, \mathcal{L})^G)_p = \operatorname{Proj} R(X, \mathcal{L})^G$$

where the first equality holds, because $k\mathcal{L}$ is very ample, the second holds because the action of G preserves gradations, and in the third we use Lemma I.2.

For the proof of (ii) by Hilbert-Nagata theorem, we know that I is generated by invariants. Since a good quotient is a locally affine quotient the map $X/\!\!/G \to Y/\!\!/G$ is an embedding. The last part of (ii) follows from [2, Thm. 5.2]. □

4. Toric varieties

A *toric variety* is a normal algebraic variety with a faithful action of a torus $(\mathbb{C}^*)^{\dim X}$ with an open, dense orbit. The classical references for this subject are [9] and [18]. An abstract toric variety can be described by a *fan* in the lattice N of one-parameter subgroups of the torus. A fan is a collection of rational, polyhedral cones, closed under taking faces and such that if two cones are in the fan, then their intersection is a face for each of them and is also in the fan. Each cone of maximal dimension corresponds to an affine patch of the toric variety.

If our toric variety is projective and we consider it together with an embedding into projective space, then the pair can be encoded by a lattice polytope, which is dual to the complete fan. The lattice points of this polytope define the coordinates of the

ambient projective space and the $\mathbb{Z}$-relations between them generate the ideal of the variety. This setting is used by Sturmfels in his book [23] and yields a generalization to not necessarily normal toric varieties, which we do not consider here.

4.1. Toric varieties in weighted projective space

The embedding of a projective toric variety X into a projective space is described by a polytope Δ with integral vertices. If we scale the polytope by an integer k, then we do not change the variety. The resulting embedding changes by composing it with k^{th} Veronese embedding. The sum of all positive multiples forms a semigroup (or a graded cone). In this situation $X = \operatorname{Proj} \bigoplus_{k\in\mathbb{N}} \mathbb{C}[k\Delta]$. When the ambient space is a weighted projective space the embedding is given by a graded cone with a set of (minimal) $\mathbb{Z}$-generators, which are no longer in the first degree. Every section of this cone determined by the grading is a rational polytope.

Definition I.7. A **weighted projective space** $\mathbb{P}(a_0, \ldots, a_n)$ with weights $(a_0, \ldots, a_n)$ where each $a_i \in \mathbb{N}$ is a positive integer is the GIT quotient of the affine space $\mathbb{C}^{n+1}$ by the action

$$t \cdot (x_0, \ldots, x_n) = (t^{a_0} \cdot x_0, \ldots, t^{a_n} \cdot x_n)$$

Again, the non-stable locus is the point $0 \in \mathbb{C}^{n+1}$.

We can assume that the greatest common divisor of the weights is one — this is by substitution $t \mapsto t^{\gcd(a_0,\ldots,a_n)}$. Let us pick integers $b_0, \ldots, b_n$ such that $\sum_{i=0}^{n} b_i \cdot a_i = 1$. The weighted projective space has the sheaf $\mathcal{O}_{\mathbb{P}}(1)$, which corresponds to the ample Weil divisor $\sum_{i=0}^{n} b_i \cdot (x_i)$, where the (x_i)'s are the divisors corresponding to the coordinates.

Weighted projective spaces are often singular. They have quotient singularities coming from finite abelian group actions.

Definition I.8. Given a lattice M, we can associate with it in a non-unique way a **graded lattice** M^{gr}, which equipped with degree map $\deg\colon M^{gr} \to \mathbb{Z}$ — the projection to the first coordinate and fits into the exact sequence

$$0 \longrightarrow M \longrightarrow M^{gr} \underset{s}{\overset{\deg}{\rightleftarrows}} \mathbb{Z} \longrightarrow 0$$

We also fix a splitting $s : \mathbb{Z} \to M^{gr}$ of the exact sequence which is equivalent to a choice of the 0 element in the $M \simeq (1, M) \subset M^{gr}$. The choice of the splitting s corresponds to a choice of linearization of the action of the torus $\mathrm{Spec}(\mathbb{C}[M^\vee)$ on itself.

Definition I.9. A **graded lattice cone** τ is a rational, convex, polyhedral cone in a graded lattice M^{gr}, with all elements having non-negative degree: $\deg(\tau) \subset \mathbb{N}$, and the zero gradation consists of one element: $\deg^{-1}(0) \cap \tau = 0$. Convex here means that $\tau \otimes_{\mathbb{Z}} \mathbb{R}_+ \subset M^{gr} \otimes_{\mathbb{Z}} \mathbb{R}$ is convex. Equivalently, τ is a (saturated) sub-semigroup of the free abelian group M^{gr} with finite set of $\mathbb{Z}$-generators all having positive degrees where the neutral element is the only one of degree zero.

Proposition I.10. *A toric variety $X \subset \mathbb{P}(a_0, \ldots, a_n)$ is described by its fan and an ample Weil divisor $\mathcal{O}_X(1)$ or equivalently by an isomorphism $X \simeq \operatorname{Proj} \mathbb{C}[\tau]$ where τ is a graded, rational, convex, polyhedral cone in a graded lattice M^{gr}. Then $\mathbb{C}[\tau] = R/I$, where R is the homogeneous coordinate ring of $\mathbb{P}(a_0, \ldots, a_n)$ and I is the homogeneous ideal of X.*

Idea of the proof. The correspondence between the ample Weil divisor and the graded cone is the following. The degree k sections of the sheaf associated to the Weil divisor form the k^{th} section of the cone τ. To go the other way, we have an isomorphism $X \simeq \operatorname{Proj} \mathbb{C}[\tau]$ and then the ample Weil divisor is $\mathcal{O}_X(1)$ — the pull-back of $\mathcal{O}_{\mathbb{P}(a_0,\ldots,a_n)}(1)$ from the ambient weighted projective space $\mathbb{P}(a_0, \ldots, a_n)$. □

The choice of the 0 element of $M \simeq (1, M) \subset M^{gr}$ in Definition I.8 is a choice of linearization of the action of the torus of X, which extends the action of the torus on itself.

Definition I.11. A **graded product** $M_1^{gr} \times_g M_2^{gr}$ of the graded lattices M_1^{gr} and M_2^{gr} is the fiber product over their degree maps, or equivalently the hyperplane $\deg_1 = \deg_2$ in the product $M_1^{gr} \times M_2^{gr}$:

$$\begin{array}{ccc} M_1^{gr} \times_g M_2^{gr} & \longrightarrow & M_2^{gr} \\ \downarrow & & \downarrow{\scriptstyle \deg_2} \\ M_1^{gr} & \xrightarrow{\deg_1} & \mathbb{Z} \end{array}$$

Definition I.12. A **graded product** $\tau_1 \times_g \tau_2$ of graded cones τ_1 and τ_2 is the fiber product over their degree map, or equivalently intersection of the hyperplane $\deg_1 = \deg_2$ with the product cone $\tau_1 \times \tau_2$:

$$\begin{array}{ccc} \tau_1 \times_g \tau_2 & \longrightarrow & \tau_2 \\ \downarrow & & \downarrow{\scriptstyle \deg_2} \\ \tau_1 & \xrightarrow{\deg_1} & \mathbb{Z} \end{array}$$

Lemma I.13. *If $\tau_1 \subset M_1^{gr}$ and $\tau_2 \subset M_2^{gr}$ are graded rational convex polyhedral cones, and*

$$X_1 = \operatorname{Proj} \mathbb{C}[\tau_1] \qquad X_2 = \operatorname{Proj} \mathbb{C}[\tau_2]$$

are corresponding projective toric varieties, then the product of these varieties under the Segre embedding

$$X_1 \times X_2 = \operatorname{Proj} \mathbb{C}[\tau_1 \times_g \tau_2]$$

corresponds to the graded product of the cones τ_1 and τ_2.

Proof. By definition $X_1 \times X_2$ under Segre embedding is equal to

$$\operatorname{Proj} \bigoplus_{i=0}^{\infty} H^0\big(X_1 \times X_2, \mathcal{O}_{X_1}(i) \boxtimes \mathcal{O}_{X_2}(i)\big).$$

For each i we know that the sections of this exterior tensor product are spanned by the product of the i^{th} graded pieces of the cones

$$H^0\big(X_1 \times X_2, \mathcal{O}_{X_1}(i) \boxtimes \mathcal{O}_{X_2}(i)\big) = \mathbb{C} \cdot \Big(\big(\tau_1 \cap \deg^{-1}(i)\big) \times \big(\tau_1 \cap \deg^{-1}(i)\big)\Big)$$

We conclude the lemma by summing the above equality over all i's to get

$$\bigoplus_{i=0}^{\infty} H^0\big(X_1 \times X_2, \mathcal{O}_{X_1}(i) \boxtimes \mathcal{O}_{X_2}(i)\big) = \mathbb{C}[\tau_1 \times_g \tau_2]$$

as required. □

4.2. Quotient of a toric variety by a subtorus

We show that the quotient of a projective toric variety $X = \operatorname{Proj} \mathbb{C}[\tau]$ by a subtorus is described by an appropriate linear section of τ.

We first recall some facts about toric varieties from [9]. If $X = \operatorname{Proj} \mathbb{C}[\tau]$, where $\tau \subset M^{gr}$ is a graded cone, then the torus of X is given by an isomorphism $\mathbb{T} = \operatorname{Hom}(M, \mathbb{Z}) \otimes_{\mathbb{Z}} \mathbb{C}^*$. The lattice $N = \operatorname{Hom}(M, \mathbb{Z})$ is the lattice of one-parameter subgroups of $\mathbb{T}$. For any subtorus $\mathbb{T}'$ of the torus $\mathbb{T}$ there are corresponding maps of lattices: the projection $M \twoheadrightarrow M'$ of the monomial lattices and the embedding $N' \hookrightarrow N$ of the lattice of one-parameter subgroups.

A linearization of the action of the torus $\mathbb{T}$ on X, induces a linearization of the action of any subtorus $\mathbb{T}' \subset \mathbb{T}$, by restricting the action. In this setting Theorem I.6 implies the following result.

Theorem I.14. *Let τ be a graded cone in a lattice M^{gr} and $X = \operatorname{Proj} \mathbb{C}[\tau]$ the*

corresponding toric variety. Let $j : \mathbb{T}' \hookrightarrow \mathbb{T}$ *be a subtorus of the torus* $\mathbb{T}$*, with* $j_* : N' \hookrightarrow N$*,* $j^* : M \twoheadrightarrow M'$ *and* $\mathrm{id} \oplus j^* : M^{gr} \to (M')^{gr}$ *the corresponding lattice maps. Then there exists a good quotient and it is equal to*

$$X /\!\!/ \mathbb{T}' = \operatorname{Proj} \mathbb{C}[\tau]^{\mathbb{T}'},$$

where

$$\mathbb{C}[\tau]^{T'} = \mathbb{C}[\tau \cap (\mathbb{Z} \oplus \ker(j^* : M \twoheadrightarrow M'))] = \mathbb{C}[\tau \cap (\mathbb{Z} \oplus N'^{\perp})].$$

Moreover the quotient $X /\!\!/ \mathbb{T}'$ *is polarized by* $\mathcal{O}_{X /\!\!/ \mathbb{T}'}(1)$ *in a natural way.*

The following example shows that we do need ample Weil divisors, not only ample line bundles.

Example I.15. Let X be the good GIT-quotient

$$\pi : \mathbb{P}^3 \times \mathbb{P}^3 \to X = \mathbb{P}^3 \times \mathbb{P}^3) /\!\!/ (\mathbb{C}^*)^3$$

of the product of two projective three-spaces by an action of three-dimensional torus acting with weights

$$\begin{bmatrix} (0 & 1 & 1 & 0) & \times & (0 & -1 & -1 & 0) \\ (0 & 1 & -1 & 0) & \times & (0 & 0 & 0 & 0) \\ (0 & 0 & 0 & 0) & \times & (0 & 1 & -1 & 0) \end{bmatrix}$$

linearized with respect to the line bundle $\mathcal{O}_{\mathbb{P}^3}(1) \boxtimes \mathcal{O}_{\mathbb{P}^3}(1)$. We will see later that $X = X(\text{⋈})$ is the model of the trivalent graph ⋈ with the first Betti number two with three edges and is a projective toric variety by Theorem I.14. The sheaf $\mathcal{O}_X(1) = \pi_*(\mathcal{O}_{\mathbb{P}^3}(1) \boxtimes \mathcal{O}_{\mathbb{P}^3}(1))$ is not a locally free $\mathcal{O}_X$-module because the associated divisor is not Cartier. To verify it we can use a computer algebra system, for example magma [3] as follows. Since any divisor on a toric variety is linearly equivalent to

a $\mathbb{T}$-invariant divisor, we identify a divisor with a corresponding $\mathbb{Z}$-combination of primitive elements of the rays of the fan. Thus we only need to check if the $\mathbb{Z}$-combination corresponding to $\mathcal{O}_X(1)$ yields a piecewise linear function on the fan, which by [18] is equivalent to our $\mathbb{T}$-invariant Weil divisor being Cartier.

CHAPTER II

PHYLOGENETIC MODELS ON TRIVALENT GRAPHS[1]

In this chapter we mention facts about graphs that we will use later, then we provide the parametric definition of the tree models. Next we recall the alternative, geometric way to define them, which yields a generalization to graphs. Lastly, we provide a way to get the toric description of the phylogenetic model from the graph.

1. Trivalent graphs

We define topological invariants of trivalent graphs and show any two graphs with the same invariants are equivalent by applying appropriate mutations, which we introduced in [5]. We *do not* assume that our graphs are connected.

Definition II.1. A **graph** $\mathcal{G}$ is set $\mathcal{V}$ of vertices and set $\mathcal{E}$ of edges together with the unordered boundary map $\partial : \mathcal{E} \to \mathcal{V}^{\otimes 2}$, where $\mathcal{V}^{\otimes 2}$ is the set of unordered pairs of vertices. We write $\partial(e) = \{\partial_1(e), \partial_2(e)\}$ and say that v is an **end of the edge** e if $v \in \partial(e)$. A vertex incident to exactly one edge is a **leaf**. The **set of leaves** is denoted by $\mathcal{L}$ and the **number of leaves** by n. If a vertex is not a leaf, it is called an **inner vertex**. An edge incident to a leaf is a **petiole** and $\mathcal{P}$ is the set of petioles. We write $\operatorname{comp}\mathcal{G}$ for the set of **connected components** of the graph and $|\operatorname{comp}\mathcal{G}|$ for the number of components. We denote by g for the **first Betti numbers** of graph, which is the rank of the first group homology of the graph viewed as a CW-complex. A graph is **trivalent** if every inner vertex has valency three. Valency of a vertex v is

[1]Part of this chapter, namely Section 2, was reprinted with permission from "Isotropic models of evolution with symmetries", by Weronika Buczyńska, Maria Donten, and Jarosław A. Wiśniewski, 2009. *Interactions of classical and numerical algebraic geometry, Contemp. Math.*, vol. 496, pp. 111–131. Copyright by Amer. Math. Soc.

the number of connected components of a sufficiently small neighborhood of v with v removed. A trivalent graph with no cycles is a **trivalent tree**.

When discussing more then one graph instead of $\mathcal{V}$, $\mathcal{E}$, n,... we will write $\mathcal{V}(\mathcal{G})$, $\mathcal{E}(\mathcal{G})$, $n(\mathcal{G})$, etc.

Remark II.2. Our graphs are *not oriented*, nevertheless we write $\partial_1(e)$ and $\partial_2(e)$ for the vertices adjacent to the edge e. This makes it easier to talk about "the other end of e".

We call the unique trivalent tree $\curlyvee$ with a single inner vertex and three leaves the **elementary tripod**. It has three edges e_1, e_2, e_3. Any trivalent graph is built of elementary tripods in the following way: given a trivalent graph $\mathcal{G}$ and any inner vertex $v \in \mathcal{V}(\mathcal{G})$ we pick a copy of elementary tripod $\curlyvee_v \simeq \curlyvee$ and an map $i_v : \curlyvee_v \to \mathcal{G}$ which sends the central vertex of $\curlyvee_v$ to v and locally near $i^{-1}(v)$ is an embedding. We present the graph $\mathcal{G}$ as a disjoint union of the graphs $\curlyvee_v$ with appropriate identification of edges

$$\mathcal{G} = \bigsqcup_{v \in \mathcal{V} \setminus \mathcal{L}} \curlyvee_v / \{ i^{-1}_{\partial_1(e)}(e) \sim i^{-1}_{\partial_2(e)}(e) \}_{e \in \mathcal{E} \setminus \mathcal{P}} \tag{II.3}$$

This construction mirrors how the model of the graph is constructed, as we will see in Definition II.16.

Example II.4. On the Figure II.1 we give an example of the above presentation of a trivalent graph for a graph with the first Betti number one and two leaves.

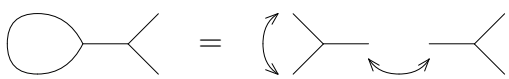


Fig. II.1.: Building a trivalent graph from tripods

Lemma II.5. *In any trivalent graph with n leaves and first Betti number g the following holds*

(i) $|\mathcal{V}|, |\mathcal{E}| \geq n$,

(ii) $2|\mathcal{E}| = 3|\mathcal{V}| - 2n$,

(iii) $|\mathcal{V}| - |\mathcal{E}| = |\operatorname{comp}\mathcal{G}| - g$.

Thus, any three of the numbers $|\mathcal{V}|$, $|\mathcal{E}|$, n, g, $|\operatorname{comp}\mathcal{G}|$ determine the other two.

Proof. To prove (ii) let us count pairs of consisting of a vertex and an adjacent edge. On one hand we will count every edge twice. On the other hand every inner vertex has three incident edges so we have $3(|\mathcal{V}| - n)$ pairs and another n pairs come from leaves which totals to $3|\mathcal{V}| - 2n$. Equation (iii) counts the Euler characteristic $|\operatorname{comp}\mathcal{G}| - g$ of the graph. □

Here we introduce operations of gluing two leaves of a graph, cutting an edge into two new edges and taking a disjoint sum of two graphs.

Definition II.6. We will use the following three constructions of trivalent graphs.

- $\mathcal{G} \sqcup \mathcal{G}'$ is the **disjoint sum** of the given graphs $\mathcal{G}$ and $\mathcal{G}'$.
- $\mathcal{G}_{l_2}^{l_1}\supset$ is the graph obtained from a given graph $\mathcal{G}$ with two distinguished leaves $l_1, l_2 \in \mathcal{L}(\mathcal{G})$ by **gluing the two leaves** l_1 and l_2, or more precisely by removing l_1 and l_2 and identifying the edge incident to l_1 with the edge incident to l_2.
- $\mathcal{G}_l \star \mathcal{G}'_{l'}$ a **graft** of given graphs $\mathcal{G}$ and $\mathcal{G}'$ each with a distinguished leaf. Figure II.2 is a schematic picture of this construction.

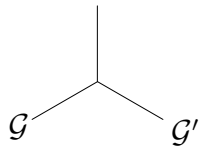


Fig. II.2.: Graft of two graphs

The new graph can be written as

$$\mathcal{G}_l \star \mathcal{G}'_{l'} = \left(\left((\mathcal{G} \sqcup \mathcal{G}')^l_{e_1} \supset\right) \sqcup \mathcal{G}'\right)^{l'}_{e_2} \supset$$

- $\mathcal{G}^e$ is the graph obtained from the given graph $\mathcal{G}$ by **cutting an internal edge** $e \in \mathcal{E}(\mathcal{G}) \setminus \mathcal{L}(\mathcal{G})$. More precisely we replace e by two new edges e_1 and e_2 with $\partial_1(e_1) := \partial_1(e)$ and $\partial_1(e_2) := \partial_2(e)$. There are two new leaves in $\mathcal{G}^e$, which are the free ends of the new edges $\partial_2(e_1)$ and $\partial_2(e_2)$.

Definition II.7. An edge $e \in \mathcal{E}$ is called a **cycle edge** if it is not a petiole and removing it does not disconnect the connected component of the graph that contains e. An edge $e \in \mathcal{E}$ is called **cycle leg** if it is incident to a cycle edge but it is not a cycle edge. A vertex $v \in \mathcal{V}$ is called **cycle vertex** if it is an end of a cycle edge. We draw example of those on Figure II.3.

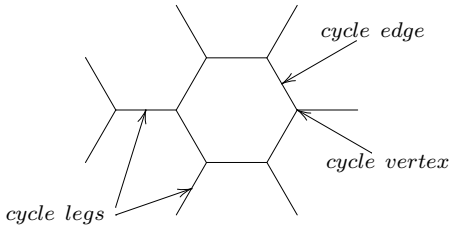


Fig. II.3.: Cycle edge, cycle leg and cycle vertex of a graph

A **path** is a sequence of distinct edges $e_0, \ldots, e_m$ with $\partial_2(e_i) = \partial_1(e_{i+1})$ for all $i \in$

$\{0, \ldots, m-1\}$, moreover $\partial_1(e_0)$ and $\partial_2(e_m)$ are both leaves or they are either equal. In the latter case, the path is called a **cycle**. Paths are **disjoint** if they have no common vertices. A **network** is a union of disjoint paths. For consistency we say that the empty set is also a network. A **cycle** is a minimal sequence of cycle edges. A cycle of length one is a **loop**. On Figure II.4 we draw examples for each those sequences.

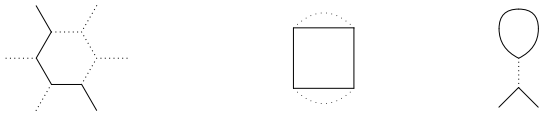


Fig. II.4.: A path, a cycle and a network containing a loop

A graph $\mathcal{G}$ is called a **polygon graph** if it has $2k$ edges of which k form the only cycle of $\mathcal{G}$ and the remaining k edges are cycle legs. If $\mathcal{G}$ is any graph, $e \in \mathcal{V}(\mathcal{G})$ a non-cycle edge and after cutting e we get a decomposition $\mathcal{G}^e = \mathcal{G}_0 \sqcup \mathcal{G}_1$ where $\mathcal{G}_1$ is a tree then we call $\mathcal{G}_1$ a **pendant tree**.

Figure II.5 shows the three trivalent trees with one internal edge e and four labeled leaves.

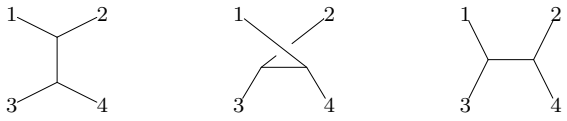


Fig. II.5.: The three trees with four labeled leaves

Let $\mathcal{G}$ be a trivalent graph and let e be an internal edge which is not a loop (the ends of e are not identified). Then a neighborhood of e in $\mathcal{G}$ is a trivalent tree with four leaves.

Definition II.8. A **mutation** of a trivalent graph $\mathcal{G}$ **along an edge** e is a graph $\mathcal{G}'$ which is obtained from $\mathcal{G}$ by removing a neighborhood of e (which is a trivalent tree with four leaves) and replacing it by one of the other trivalent trees from Figure II.5. Two graphs are **mutation-equivalent** if they may be transformed by sequence of mutations into each other.

Remark II.9. By definition it is not possible to mutate along an edge that forms a cycle of length one. However, for longer cycles, mutations are possible, and one shortens the length of the cycle. Figure II.6 shows this fenomena for Hammock graph mutation equivalent to LittleMan.

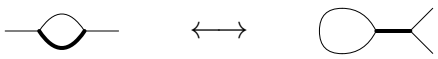


Fig. II.6.: Mutation along cycle edge shortens a cycle

Lemma II.10. *Suppose edges* $\{e_1, \ldots, e_k\}$ *form a cycle in the graph* $\mathcal{G}$ *and assume* $k > 1$. *Then, for any* $i \in \{1, \ldots, k\}$ *one of the two mutations along* e_i *shortens the cycle* $\{e_1, \ldots, e_k\}$ *by one in the resulting graph, i.e.* $\{e_1, \ldots, e_{i-1}, e_{i+1}, \ldots, e_k\}$ *is a cycle in the new graph.*

A **caterpillar** is a trivalent tree, which after removing all leaves and petioles becomes a string of edges as shown on Figure II.7.

Fig. II.7.: Caterpillar tree

Lemma II.11. *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be connected, trivalent graphs both with n leaves and first Betti numbers g. Then they are mutation-equivalent. Moreover, for any ordered subsets S_1 of cycle edges of $\mathcal{G}_1$ and S_2 of cycle edges of $\mathcal{G}_2$, of the same size, both with the property that removing S_i from $\mathcal{G}_i$ does not disconnect the graph, we can find a sequence of mutations that avoid the edges from S_1 (S_2) and sends i^{th} edge of S_1 to the i^{th} edge of S_2. Also, any mutation sends a leaf of $\mathcal{G}_1$ to a leaf of $\mathcal{G}_2$.*

Proof. Let $\mathcal{G}$ be connected, trivalent graph with n leaves and the first Betti number g and S a subset of cycle edges as above. We will prove that $\mathcal{G}$ is mutation-equivalent to a trivalent graph obtained by attaching g cycles of length one to a caterpillar tree with $n+g$ leaves. We will choose mutations so that they will satisfy the required property.

Step 1. We proceed by induction on the set S and the first Betti number of $\mathcal{G}$. For an edge $e \in S$ we can find a cycle that contains no other elements of S. This is because after removing all edges from S the graph $\mathcal{G}$ is connected, so there is a path γ from $\partial_1(e)$ to $\partial_2(e)$, which together with e form the required cycle. By repeatedly using Lemma II.10, we reduce the length of this cycle to one, by performing mutations along edges from γ. In the new graph the edge e forms a loop. We can consider this graph with e removed, reducing both the size of S and g. If $|S| < g$, then we repeat the above $g - |S|$ times starting from any cycle edge, which is not a loop.

After repeating this procedure g times, we get a tree with g loops (all edges from S are among them) attached to some leaves. We can assume that this tree is a caterpillar, as we know from [5, Lem. 2.18], that any trivalent tree is mutation-equivalent to a caterpillar with the same number of leaves.

Step 2. We observe that it does not matter to which leaves the cycles are attached, we can move a cycle from a leaf to any another leaf.

In Figure II.8 we illustrate those two steps.

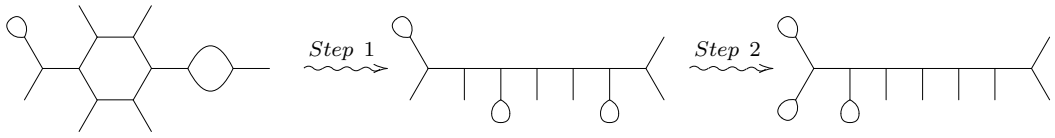


Fig. II.8.: Every graph is mutation-equivalent to a caterpillar graph

The last claim follows simply form the definition: mutation maps an inner edge to an inner edge, and a leaf to a leaf. □

2. Parametrization of tree models

From the point of view of algebraic geometry, phylogenetic trees encode certain linear subsystems of the Segre system on the product of projective spaces. In the case of binary symmetric models of trivalent trees these are subsystems of sections of Segre system on a product of $\mathbb{P}^1$'s invariant with respect to some $\mathbb{Z}_2^{|\mathcal{E}\setminus\mathcal{L}|}$ action.

Notation II.12. Let W be a finite dimensional, complex vector space with a distinguished basis, sometimes called letters: $\{\alpha_0, \alpha_1, \alpha_2, \dots\}$. We consider the map $\sigma : W \to \mathbb{C}$, such that $\sigma(\alpha_i) = 1$ for every i, that is $\sigma = \sum \alpha_i^*$.

Let $\widehat{W}$ be a subspace of the second tensor product $W \otimes W$. An element $\sum_{i,j} a_{ij}(\alpha_i \otimes \alpha_j)$ of $\widehat{W}$ can be represented as a matrix (a_{ij}). We will assume that $\widehat{W}$ is contained in the second symmetric power $S^2(W)$, so these matrices are symmetric.

Given a tree $\mathcal{T}$ and a vector space W, and a subspace $\widehat{W} \subset S^2W$, we associate to any vertex v of $\mathcal{V}(\mathcal{T})$ a copy of W denoted by W_v and for any edge $e \in \mathcal{E}(\mathcal{T})$ we associate a copy of $\widehat{W}$ understood as the subspace in the tensor product $\widehat{W}^e \subset W_{\partial_1(e)} \otimes W_{\partial_2(e)}$. Note that although the pair $\{\partial_1(e), \partial_2(e)\}$ is unordered, this definition

makes sense since $\widehat{W}$ consists of symmetric tensors. Elements of $\widehat{W}^e$ will be written as symmetric matrices $(a^e_{\alpha_i,\alpha_j})$.

Definition II.13. A triple $(\mathcal{T}, W, \widehat{W})$ together with the above association is called a symmetric, unrooted phylogenetic tree.

Construction II.14. Let us consider a linear map of tensor products

$$\widehat{\Psi} : \widehat{W}^{\mathcal{E}} = \bigotimes_{e\in\mathcal{E}} \widehat{W}^e \longrightarrow W_{\mathcal{V}} = \bigotimes_{v\in\mathcal{V}} W_v$$

defined by setting its dual as follows

$$\widehat{\Psi}^*(\otimes_{v\in\mathcal{V}} \ \alpha_v^*) = \otimes_{e\in\mathcal{E}} \ (\alpha_{\partial_1(e)} \otimes \alpha_{\partial_2(e)})^*_{|\widehat{W}^e}$$

where α_v stands for an element of the chosen basis $\{\alpha_i\}$ of the space W_v. The **complete affine geometric model** of the phylogenetic tree $(\mathcal{T}, W, \widehat{W})$ is the image of the associated multi-linear map

$$\widetilde{\Psi} : \prod_{e\in\mathcal{E}} \widehat{W}^e \longrightarrow W_{\mathcal{V}} = \bigotimes_{v\in\mathcal{V}} W_v$$

The induced rational map of projective varieties will be denoted by Ψ:

$$\Psi : \prod_{e\in\mathcal{E}} \mathbb{P}(\widehat{W}^e) \ \dashrightarrow \mathbb{P}(W_{\mathcal{V}}) = \mathbb{P}(\bigotimes_{v\in\mathcal{V}} W_v)$$

and the closure of the image of Ψ is called the **complete projective geometric model**, or just the complete model of $(\mathcal{T}, W, \widehat{W})$. The maps $\widetilde{\Psi}$ and Ψ are called the parametrization of the respective model.

We can hide any set of vertices by applying the contraction map $\sigma = \sum_i \alpha_i^*$ to their tensor factors. In what follows will hide inner nodes and project to leaves. That

is, we consider the map

$$\Pi_{\mathcal{L}} : W_{\mathcal{V}} = \bigotimes_{v\in\mathcal{V}} W_v \to W_{\mathcal{L}} = \bigotimes_{v\in\mathcal{L}} W_v$$

$$\Pi_{\mathcal{L}} = (\otimes_{v\in\mathcal{L}}\ id_{W_v}) \otimes (\otimes_{v\in\mathcal{E}\setminus\mathcal{L}}\ \sigma_{W_v})$$

Definition II.15. The affine geometrical model of a phylogenetic tree $(\mathcal{T}, W, \widehat{W})$ is the affine subvariety of $W_{\mathcal{L}} = \bigotimes_{v\in\mathcal{L}} W_v$ which is the image of the composition $\Phi = \Pi_{\mathcal{L}} \circ \Psi$. Respectively, the **projective geometrical model**, or just the model, denoted by $X(\mathcal{T})$ is the underlying projective variety in $\mathbb{P}(W_{\mathcal{L}})$. For $X = X(\mathcal{T})$, by $\mathcal{O}_X(1)$ we denote the line bundle coming from the embedding in the projective space $\mathbb{P}(W_{\mathcal{L}})$.

Note that $X(\mathcal{T})$ is the closure of the image of the respective rational map

$$\prod_{e\in\mathcal{E}} \mathbb{P}(\widehat{W}^e) \dashrightarrow \mathbb{P}\left(\bigotimes_{v\in\mathcal{L}} W_v\right)$$

which is defined by a special linear subsystem $\left|\bigotimes_{e\in\mathcal{E}} p^*_{\mathbb{P}(\widehat{W}^e)}\mathcal{O}_{\mathbb{P}(\widehat{W}^e)}(1)\right|$ in the Segre linear system, where $p^*_{\mathbb{P}(\widehat{W}^e)}$ is the projection from the product to the respective component. We will call this map a **rational parametrization** of the model.

The above definition of parametrization is an unrooted and algebraic version of what is commonly considered in the statistics literature, see [1], [24] or [6].

3. Phylogenetic model of a graph

The phylogenetic model of a trivalent graph is a generalization of the discussed projective geometrical model of a binary symmetric model on a trivalent tree. Graph models no longer have a parametrization — we generalize the alternative construction given in [5] which uses quotients. In Section 3.1 we describe the quotient construction

so that it is valid for both trees and graphs. Then in Section 3.2 we provide a description of lattice and cone of the resulting toric variety and we prove that it yields the phylogenetic model.

3.1. Definition as quotient

Given a not necessarily connected trivalent graph $\mathcal{G}$, we construct a toric variety $X(\mathcal{G})$, generalizing the binary symmetric model of trivalent tree from [5].

As we have already explained, see equation (II.3), any trivalent graph is the union of $|\mathcal{V}| - n$ elementary tripods with some edges identified. To define the variety $X(\mathcal{G})$ we replace each elementary tripod $\curlyvee_v$ with $\mathbb{P}^3_v$, union with product, and the edge identification with a quotient by an action of a one-parameter torus.

Definition II.16. Let $\mathcal{G}$ be a trivalent graph. To an inner vertex $v \in \mathcal{V} \setminus \mathcal{L}$ we associate projective space $\mathbb{P}^3_v$ with coordinates $x^v_\emptyset, x^v_{12}, x^v_{13}, x^v_{23}$. To any edge $e \in \mathcal{E}$ we associate an action λ^e_v of $\mathbb{C}^*$ on $\mathbb{P}^3_v$ with weights 0 and 1 as follows:

$$\lambda^e_v(t)(x_S) = \begin{cases} t \cdot x^v_S & \text{if the index of } i_v^{-1}(e) \in \{e_1, e_2, e_3\} \text{ belongs to the set } S, \\ x^v_S & \text{otherwise.} \end{cases}$$

So we have an action of a three-dimensional torus on $\mathbb{P}^3 = \operatorname{Proj} \mathbb{C}[x^v_\emptyset, x^v_{12}, x^v_{13}, x^v_{23}]$ with weights:

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

In other words if for example $i_v(e_2) = e$ then λ^e_v acts with weight 1 on x^v_{12} and x^v_{23} and with weight 0 on $x^v_\emptyset$ and x^v_{13}. This action extends to an action λ^e_v on $\prod_{v \in \mathcal{V} \setminus \mathcal{L}} \mathbb{P}^3_v$ which is non-trivial only if v is an end of the edge e. Thus, for any internal edge

$e \in \mathcal{E} \setminus \mathcal{P}$, we can define a $\mathbb{C}^*$-action $\lambda^e_{\partial_1(e)} \times -\lambda^e_{\partial_2(e)}$ on

$$\prod_{v \in \mathcal{V} \setminus \mathcal{L}} \mathbb{P}^3_v \tag{II.17}$$

to be the product action of the action $\lambda^e_{\partial_1(e)}$ on $\mathbb{P}^3_{\partial_1(e)}$ and the action $\lambda^e_{\partial_2(e)}$ with opposite weights on $\mathbb{P}^3_{\partial_2(e)}$. We define the **phylogenetic model of a trivalent graph** $\mathcal{G}$ to be the good quotient:

$$X(\mathcal{G}) := \Big(\prod_{v \in \mathcal{V} \setminus \mathcal{L}} \mathbb{P}^3_v \Big) \quad /\!\!/ \prod_{e \in \mathcal{E} \setminus \mathcal{P}} \big(\lambda^e_{\partial_1(e)} \times -\lambda^e_{\partial_2(e)} \big) \tag{II.18}$$

of the toric variety $\prod_{v \in \mathcal{V} \setminus \mathcal{L}} \mathbb{P}^3_v$ by a subtorus of dimension $|\mathcal{E}| - |\mathcal{L}|$ of the torus. The subtorus by which we are dividing is a product of all the $\mathbb{C}^*$'s over all internal edges of the graph $\mathcal{G}$ and the linearized line bundle is $\boxtimes_{v \in \mathcal{V}(\mathcal{G})} \mathcal{O}_{\mathbb{P}^3_v}(1)$. By Theorem I.14. $X(\mathcal{G})$ is toric as it is the quotient of a toric variety by a subtorus.

Remark II.19. In Definition (II.18) the choice that we made defining the action of the torus $(\mathbb{C}^*)^{\mathcal{V} \setminus \mathcal{L}}$ only depends on the choice of coordinates of the torus. If we choose different orientation of the edge e, then the two $\mathbb{C}^*$-actions $\lambda^e_{\partial_1(e)} \times -\lambda^e_{\partial_2(e)}$ and $-\lambda^e_{\partial_1(e)} \times \lambda^e_{\partial_2(e)}$ differ by composing with $t \mapsto \frac{1}{t}$.

Remark II.20. Let l be a leaf of a graph $\mathcal{G}$ and e the adjacent petiole. The action λ^e_l descends to a non-trivial action on the quotient variety $X(\mathcal{G})$ and is denoted by λ^l. For a subset $\mathcal{S} \subset \mathcal{L}$ of the leaves of $\mathcal{G}$ of cardinality k we have an action of a k-dimensional torus $\mathbb{T}(\mathcal{S})$ — a product of the corresponding λ^l's.

If we set $k = |\mathcal{V}| - n$ the number of inner vertices, we can rewrite $|\mathcal{V}| - |\mathcal{E}| = |\operatorname{comp} \mathcal{G}| - g$ using Lemma II.5(ii) to get $k = (2g - 2|\operatorname{comp} \mathcal{G}|) + n$. Observe that

- k is the number of the $\mathbb{P}^3$'s in (II.17)
- g is the first Betti number.

On the other hand, $|\mathcal{E}| - n = k + g - |\operatorname{comp}\mathcal{G}|$ is the number of inner edges which is the dimension of the torus that we divide by in (II.18). We get a variety of dimension

$$\dim X(\mathcal{G}) = 3k - (|\mathcal{E}| - n) = 3g - 3|\operatorname{comp}\mathcal{G}| + 2n = |\mathcal{E}|.$$

3.2. Lattice and cone

Given a trivalent graph $\mathcal{G}$ we construct the toric data that allows to recover its toric model. The graded lattice, denoted by M^{gr}, as well as the graded cone in it have both rank one bigger than the dimension of the model $X(\mathcal{G})$, and the latter is equal to the number of edges $\mathcal{E}(\mathcal{G})$.

Definition II.21. Given a graph $\mathcal{G}$ let $\mathbb{Z}\mathcal{E} = \bigoplus \mathbb{Z} \cdot e$ be the lattice spanned by $\mathcal{E}$, and $\mathbb{Z}\mathcal{E}^\vee = \operatorname{Hom}(\mathbb{Z}\mathcal{E}, \mathbb{Z})$ be its dual. Elements of the lattice $\mathbb{Z}\mathcal{E}$ are formal linear combinations of the edges, forming the standard basis of $\mathbb{Z}\mathcal{E}$. The dual lattice $\mathbb{Z}\mathcal{E}^\vee$ comes with the dual basis $\{e^*\}_{e\in\mathcal{E}}$. We identify vertices of the graph $\mathcal{G}$ with certain elements of $\mathbb{Z}\mathcal{E}^\vee$:

$$v = \sum_{e \ni v} e^*. \tag{II.22}$$

We also define $M = \{u \in \mathbb{Z}\mathcal{E} : \forall v \in \mathcal{V}\ v(u) \in 2\mathbb{Z}\}$ and its dual $N = \operatorname{Hom}(M, \mathbb{Z})$. Then the graded lattice of the graph is

$$M^{gr} = \mathbb{Z} \oplus M,$$

with the degree map

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

which is the projection to the first summand. The **degree** of $\omega \in M^{gr}$ is $\deg(w)$.

If there is more then one graph in question we will write $M(\mathcal{G})$ for $M^{gr}(\mathcal{G})$ etc.

Let us use the following notation for the elements of the lattice $\mathbb{Z}\mathcal{E}^\vee$ dual to the

edges meeting at the vertex v

$$a_v := \big(i_v(e_1)\big)^*, \quad b_v := \big(i_v(e_2)\big)^*, \quad c_v := \big(i_v(e_3)\big)^*,$$

where $\{e_1, e_2, e_3\}$ are the edges of $\curlywedge$ and $i_v : \curlywedge \hookrightarrow \mathcal{G}$ is, as before, a map which is locally an embedding and sends the central vertex of the $\curlywedge$ to v — an inner vertex of $\mathcal{G}$. Whenever we use this notation we have a fixed presentation as in (II.3).

Given an element ω in either $\mathbb{Z}\mathcal{E}$, M or M^{gr}, each of $a_v, b_v, c_v \in \mathbb{Z}\mathcal{E}^\vee$ measures the coefficient of ω at an edge incident to v. Then (II.22) becomes

$$v = a_v + b_v + c_v.$$

Definition II.23. The **degree** of $\omega \in M^{gr}$ **at a vertex** $v \in \mathcal{V}(\mathcal{G})$ is

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

The **minimal degree** of ω is

$$\deg_{\min}(\omega) := \max_{v \in \mathcal{V}}\{\deg_v(\omega)\},$$

where $\pi_M : M^{gr} \to M$ is the projection to the second summand.

The name minimal degree will be clear after we define the cone $\tau(\mathcal{G})$.

We identify paths and networks in $\mathcal{G}$ with elements of the lattices M and M^{gr}, by replacing union with sum in the group $\mathbb{Z}\mathcal{E}$

Definition II.24. A **network in the graded lattice** M^{gr} is a pair $\omega = (1, a) \in M^{gr}$ where $a \in M$ is a network.

Lemma II.25. *An element of the lattice M is represented by a labeling of the edges of $\mathcal{G}$ with integers so that the sum at any vertex is even. Thus the lattice $M \subset \mathbb{Z}\mathcal{E}$ is generated by*

(i) networks

(ii) $\{2e \mid e \in \mathcal{E}\}$.

Proof. Let $\omega \in M$. By using generators of the second type, we can assume that $0 \leq a_v(\omega), b_v(\omega), c_v(\omega) \leq 1$ for any vertex v. This implies that $a_v(\omega) + b_v(\omega) + c_v(\omega)$ equals 0 or 2 and either two among $a_v(\omega), b_v(\omega), c_v(\omega)$ are one or all are zero. This implies that ω is a network, since it corresponds to a disjoint union of path. A path goes through a vertex v means in terms of $a_v(\omega), b_v(\omega), c_v(\omega)$ that exactly two of them are one. □

We define the cone $\tau(\mathcal{G})$ of the graph, which is the semigroup defining the model of the graph as projective spectrum of the semigroup ring, as we will see in Theorem II.28.

Definition II.26. For a graph $\mathcal{G}$ we define its cone $\tau = \tau(\mathcal{G}) \subset M^{gr}$ as the set of $\omega \in M^{gr}$ which satisfy following inequalities:

(i) $a_v(\omega), b_v(\omega), c_v(\omega) \geq 0$,

(ii) for any vertex $v \in \mathcal{V}$ triangle inequalities hold

$$|a_v(\omega) - b_v(\omega)| \leq c_v(\omega) \leq a_v(\omega) + b_v(\omega), \text{ and}$$

(iii) $\deg(\omega) \geq \deg_{\min}(\omega)$.

Remark II.27. To explain the name minimal degree $\deg_{\min}(\omega)$, note that for any ω in the cone we have the following equality

$$\deg_{\min}(\omega) = \min_{\omega' \in \tau}\{\deg(\omega') : \pi_{\widehat{M}}(\omega') = \pi_{\widehat{M}}(\omega)\}.$$

Proof of the remark. By part (iii) of the Definition II.26 of τ for any $\omega' \in \tau$

satisfying $\pi_{\widehat{M}}(\omega') = \pi_{\widehat{M}}(\omega)$ we have

$$\deg(\omega') \geq \deg_{\min}(\omega') = \deg_{\min}(\omega)$$

since by definition of $\deg_{\min}(\omega)$ only depends on $\pi_{\widehat{M}}(\omega)$. This means

$$\deg_{\min}(\omega) \leq \min_{\omega' \in \tau}\{\deg(\omega') : \pi_{\widehat{M}}(\omega') = \pi_{\widehat{M}}(\omega)\}.$$

To prove the equality we will find $\omega' \in \tau$ with $\deg(\omega') = \deg_{\min}(\omega)$. Let us write $\omega = (\deg(\omega), \alpha)$ as it is an element of M^{gr}. Recall that $\deg_{\min}(\omega)$ is the maximum of $\deg_v(\omega) = \frac{1}{2}\cdot(a_v+b_v+c_v)(w)$ over all vertices v of the graph. Thus $\omega' = (\deg_{\min}(\omega), \alpha)$ is in the cone τ and has the required degree in M^{gr}. □

Theorem II.28. *The variety $X(\mathcal{G})$ is isomorphic to the toric variety* $\operatorname{Proj}\mathbb{C}[\tau(\mathcal{G})]$.

Proof. To see this we first observe that each $\mathbb{P}^3_v$ in Definition II.16 of the model $X(\mathcal{G})$ can be written as $\operatorname{Proj}\mathbb{C}[\tau(\curlywedge_v)]$, where each cone

$$\tau(\curlywedge_v) = \operatorname{conv}(0000, 1000, 1110, 1101, 1011)$$

is a cone over a tetrahedron and is clearly defined by the required inequalities. Next, taking the product of $\mathbb{P}_v$ corresponds by Lemma I.13 to taking a graded product of cones. Thus the product cone is defined by required inequalities. Lastly we use the description of the quotient of a toric variety by a subtorus of the torus in Theorem I.14. The subtorus in Definition II.16 is a product of the $\mathbb{C}^*_e$ over all internal edges. Taking the quotient with respect to such a torus corresponds to cutting the cone with the hyperplane of the type $a_{\partial_1(e)} = b_{\partial_2(e)}$, which preserves the inequalities. □

3.3. $\mathbb{Z}$-generators of the cone $\tau(\mathcal{G})$

Knowing that the model $X(\mathcal{G})$ is the projective spectrum of the semigroup algebra of $\tau(\mathcal{G})$ means that it is a subvariety of a weighted projective space with weights equal to the degrees of the chosen generators. When $\mathcal{G} = \mathcal{T}$ is a tree the cone is generated in degree 1 so the embedding is into a (straight) projective space $\mathbb{P}^k = \mathbb{P}(1, \ldots, 1)$. In this case, by [5], we already know all about this cone, see Proposition II.36 below. It is represented by its degree 1 section — a normal lattice polytope $\Delta(\mathcal{T}) \subset 1 \times M$, whose vertices span the cone $\tau(\mathcal{T})$ and the lattice points generate the semigroup. Our goal is to show that for graphs with the first Betti number one, the semigroup is generated in degrees 1 and 2.

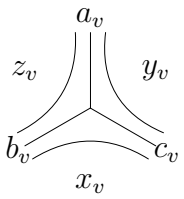
In order to describe $\mathbb{Z}$-generators of the cone $\tau(\mathcal{G})$ we will express elements of $\tau(\mathcal{G})$ in terms of $\mathcal{G}$. We also decompose the graph $\mathcal{G}$ into smaller graphs for which $\mathbb{Z}$-generators of the corresponding cones are easier to find.

We explain that any element ω of the cone $\tau(\mathcal{G})$ locally decomposes into paths. In the graph $\curlywedge$ there are three non-empty paths, each consisting of two edges. Let us 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 $\curlywedge$.

For an arbitrary $\mathcal{G}$, we know that given an element $\omega \in \tau(\mathcal{G})$ of the cone and a vertex $v \in \mathcal{V}(\mathcal{G})$, the numbers $a_v(\omega), b_v(\omega), c_v(\omega)$ satisfy the triangle inequalities and their sum is even. This allows us to, locally at v, rewrite ω as sum of paths x, y and z. The picture of this decomposition is drawn in Figure II.9.



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

Fig. II.9.: Local paths around a vertex

Our aim is to find the $\mathbb{Z}$-generators by understanding how the graph $\mathcal{G}$ was built from smaller pieces. Each of the operations in Definition II.6 has a corresponding operation on lattices and cones. By Definition II.16, the model of a disjoint sum of graphs is the product of the models, so the underlying cone is the graded product of corresponding cones.

Lemma II.29. *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two trivalent graphs then*

$$\begin{aligned} M^{gr}(\mathcal{G}_1 \sqcup \mathcal{G}_2) &= M^{gr}(\mathcal{G}_1) \times_g M^{gr}(\mathcal{G}_2), \text{ and} \\ \tau(\mathcal{G}_1 \sqcup \mathcal{G}_2) &= \tau(\mathcal{G}_1) \times_g \tau(\mathcal{G}_2). \end{aligned}$$

In the definition of $X(\mathcal{G})$ we take a quotient by a torus corresponding to the set of inner edges. In other words we have translated the operation of gluing of two leaves of a graph $\mathcal{G}$ into taking a quotient by appropriate $\mathbb{C}^*$-action of the model $X(\mathcal{G})$. The following observation says that if we choose to glue some pairs of leaves first and then the rest of the pairs it does not matter how we partition the set of pairs of leaves or which order we choose. In all cases the resulting variety is the same.

Lemma II.30. *Let two reductive, commutative groups H_1 and H_2 and their direct sum $H_1 \oplus H_2$ act on a projective variety X. Suppose all those actions are linearized with respect to some ample Weil divisor $\mathcal{L}$. Then*

$$X/\!\!/(H_1 \oplus H_2) = (X/\!\!/H_1)/\!\!/H_2 = (X/\!\!/H_2)/\!\!/H_1,$$

where the semistable points on X are taken with respect to $\mathcal{L}$ and on quotients of X with respect to the push-forward of $\mathcal{L}$.

We have identified the vertices of $\mathcal{G}$ with elements of $\mathbb{Z}\mathcal{E}^\vee$, see (II.22). We observed in Remark II.20 that a leaf l yields a $\mathbb{C}^*$-action λ^l on $X(\mathcal{G})$. Given two leaves l_1 and l_2 of $\mathcal{G}$, by definition we have

$$X(\mathcal{G}_{l_2}^{l_1}\supset) = X(\mathcal{G})/\!\!/ \left(\lambda^{l_1} \times -\lambda^{l_2}\right).$$

In terms of toric geometry this quotient corresponds to the intersection of $\tau(\mathcal{G})$ with the kernel of $l_1 - l_2$, where we treat l_1 and l_2 as elements of the lattice $(M^{gr})^\vee$. Thus the following lemma is a consequence of Theorem I.14.

Lemma II.31. *Let l_1 and l_2 be distinct leaves of $\mathcal{G}$. Then*

$$\begin{aligned} M^{gr}(\mathcal{G}_{l_2}^{l_1}\supset) &= M^{gr}(\mathcal{G}) \cap \ker(l_1 - l_2) \\ \tau(\mathcal{G}_{l_2}^{l_1}\supset) &= \tau(\mathcal{G}) \cap \ker(l_1 - l_2). \end{aligned}$$

The reverse operation on graphs is to cut an edge into two new edges. In the next lemma we explain how this is reflected on the cones and lattices.

Lemma II.32. *Let $\mathcal{G}$ be a trivalent graph and $e \in \mathcal{E}\backslash\mathcal{P}$ an internal edge. As before $\mathcal{G}^e$ is the graph obtained from $\mathcal{G}$ by cutting the edge e. Then there are natural embeddings of the cones and graded lattices:*

$$i^e : M^{gr}(\mathcal{G}) \hookrightarrow M^{gr}(\mathcal{G}^e) \qquad\qquad i^e : \tau(\mathcal{G}) \hookrightarrow \tau(\mathcal{G}^e)$$

Proof. Let

$$\mathbb{Z}\mathcal{E}^e(\mathcal{G}) = \bigoplus_{e' \in \mathcal{E}(\mathcal{G})\backslash\{e\}} \mathbb{Z} \cdot e'$$

be the lattice spanned by all other edges. We can decompose the lattices $(\mathbb{Z}\mathcal{E})^{gr}(\mathcal{G})$

and $(\mathbb{Z}\mathcal{E})^{gr}(\mathcal{G}^e)$

$$\mathbb{Z}\mathcal{E}(\mathcal{G}) = \mathbb{Z} \oplus \mathbb{Z}\mathcal{E}^e(\mathcal{G}) \oplus \mathbb{Z} \cdot e,$$
$$\mathbb{Z}\mathcal{E}(\mathcal{G}^e) = \mathbb{Z} \oplus \mathbb{Z}\mathcal{E}^e(\mathcal{G}) \oplus \mathbb{Z} \cdot e_1 \oplus \mathbb{Z} \cdot e_2.$$

Thus we can embed the lattices identifying the first two summands and taking a diagonal embedding of the third one: $i^e := \mathrm{id}_{\mathbb{Z}} \oplus \mathrm{id}_{\mathbb{Z}\mathcal{E}^e} \oplus \Delta_{\mathbb{Z}} : (\mathbb{Z}\mathcal{E})^{gr}(\mathcal{G}) \hookrightarrow (\mathbb{Z}\mathcal{E})^{gr}(\mathcal{G}^e)$. To complete the proof we check that i^e restricts to the lattices with parity condition and to the cones.

$$\begin{array}{ccc} \mathbb{Z}\mathcal{E}(\mathcal{G}) & \xhookrightarrow{i^e} & \mathbb{Z}\mathcal{E}(\mathcal{G}^e) \\ \uparrow & & \uparrow \\ M^{gr}(\mathcal{G}) & \xhookrightarrow{i^e} & M^{gr}(\mathcal{G}^e) \end{array} \qquad \begin{array}{ccc} \mathbb{Z}\mathcal{E}(\mathcal{G}) & \xhookrightarrow{i^e} & \mathbb{Z}\mathcal{E}(\mathcal{G}^e) \\ \uparrow & & \uparrow \\ \tau(\mathcal{G}) & \xhookrightarrow{i^e} & \tau(\mathcal{G}^e) \end{array}$$

To see it we only need to check the parity condition about the ends $\partial_1(e)$ and $\partial_2(e)$ of the edge e that we cut. By definition $e_1^*(i^e(e)) = e_2^*(i^e(e))$, so for any $\omega \in M^{gr}$ we have $\partial_1(e)(\omega) = \partial_1(e_1)(i^e(\omega))$ and $\partial_2(e)(\omega) = \partial_2(e_2)(i^e(\omega))$. In the same way i^e preserves all the inequalities defining cones $\tau(\mathcal{G})$ and $\tau(\mathcal{G}^e)$. □

When the edge e is not a cycle edge, the graph $\mathcal{G}^e$ is not connected. We write $\mathcal{G}^e = \mathcal{G}_1 \sqcup \mathcal{G}_2$, where $\mathcal{G}_1$ (respectively $\mathcal{G}_2$) is the part containing e_1 (respectively e_2). Then we have a projection π_1^e (respectively π_2^e) of lattices

$$\pi_1^e : M^{gr}(\mathcal{G}^e) = M^{gr}(\mathcal{G}_1) \times M^{gr}(\mathcal{G}_2) \twoheadrightarrow M^{gr}(\mathcal{G}_1)$$

which restricts to a projection of cones. For a non-cycle edge $e \in \mathcal{E}$ we denote by ρ_1^e (respectively ρ_2^e) the composition $\rho_1^e = \pi_1^e \circ i^e$ of the above defined maps.

Remark II.33. When $e \in \mathcal{E}$ is not a cycle edge we write $\mathcal{G}^e = \mathcal{G}_1 \sqcup \mathcal{G}_2$. Then the cone $\tau(\mathcal{G})$ is the following fiber product of the cones $\rho_1^e(\tau(\mathcal{G})) = \tau(\mathcal{G}_1)$ and $\rho_2^e(\tau(\mathcal{G})) =$

$\tau(\mathcal{G}_2)$. The same is true for the lattice $M^{gr}(\mathcal{G})$.

$$\begin{array}{ccc} \tau(\mathcal{G}) & \xrightarrow{\rho_1^e} & \tau(\mathcal{G}_1) \\ \downarrow{\scriptstyle \rho_2^e} & & \downarrow{\scriptstyle \deg \oplus e_1^*} \\ \tau(\mathcal{G}_2) & \xrightarrow{\deg \oplus e_2^*} & \mathbb{Z} \oplus \mathbb{Z} \end{array} \qquad \begin{array}{ccc} M^{gr}(\mathcal{G}) & \xrightarrow{\rho_1^e} & M^{gr}(\mathcal{G}_1) \\ \downarrow{\scriptstyle \rho_2^e} & & \downarrow{\scriptstyle \deg \oplus e_1^*} \\ M^{gr}(\mathcal{G}_2) & \xrightarrow{\deg \oplus e_2^*} & \mathbb{Z} \oplus \mathbb{Z} \end{array}$$

Now we turn our attention to our main task of finding the $\mathbb{Z}$-generators of the cone $\tau(\mathcal{G})$.

Lemma II.34. *For any graph $\mathcal{G}$ the set of degree 1 integer points of cone $\tau(\mathcal{G})$ is equal to the set of networks.*

Proof. If $\omega \in \tau$ is a point in the cone of degree 1, then for any vertex $v \in \mathcal{V}$,

$$1 = \deg(\omega) \geq \deg_{\min}(\omega) = \max_{u \in \mathcal{V}}\{\deg_u(\omega)\} \geq \deg_v(\omega) \geq 0.$$

By definition $\deg_v = x_v + y_v + z_v \geq 0$ so exactly one of $x_v(\omega)$, $y_v(\omega)$, $z_v(\omega)$ equals one and the other two are zero or all are zero. Equivalently exactly two of $a_v(\omega)$, $b_v(\omega)$, $c_v(\omega)$ are one, and the third one is zero, or all are zero. This means that ω is a network. □

Corollary II.35. *All networks are among the minimal $\mathbb{Z}$-generators of the cone $\tau(\mathcal{G})$.*

In fact when the graph in question is a tree these are the $\mathbb{Z}$-generators.

Proposition II.36 ([5, §2.1])**.** *If $\mathcal{G}$ is a trivalent tree, then $\tau(\mathcal{G})$ is generated in degree 1. Moreover, the generators are exactly networks of paths, which in this case are determined by their values on the leaves. Thus a generator of $\tau(\mathcal{G})$ is identified with a sequence of 0's and 1's of length $n(\mathcal{G})$ with even number of 1's. As a consequence a model of a trivalent tree with n leaves comes with an embedding into projective space $\mathbb{P}^{2^{n-1}-1}$.*

Let $\mathcal{G}$ be a graph with the first Betti number one. We will describe the generators of the semigroup $\tau(\mathcal{G})$ in this case. We cut all the cycle legs $l_1, \ldots, l_k$ of $\mathcal{G}$ and write $\mathcal{G}^{l_1,\ldots,l_k} = \mathcal{G}_0 \sqcup \mathcal{G}_1 \sqcup \ldots \sqcup \mathcal{G}_k$, where $\mathcal{G}_0$ is a polygon graph and thus $\mathcal{G}_1, \ldots, \mathcal{G}_k$ are pendant trees (see Definition II.7). Thus any element $\omega \in \tau(\mathcal{G})$ has a lift $\tilde{\omega} \in \tau(\mathcal{G}_0 \sqcup \ldots \sqcup \mathcal{G}_k) = \tau(\mathcal{G}_0) \times_g \tau(\mathcal{G}_1) \times_g \ldots \times_g \tau(\mathcal{G}_k)$ and **components** $\tilde{\omega} = (\omega_0, w_1, \ldots, \omega_k)$, which can be written $\omega_i = \rho^{l_i}(\omega)$.

Theorem II.37. *Let $\mathcal{G}$ be a trivalent graph with the first Betti number exactly one. Any element $\omega \in M^{gr}(\mathcal{G})$ is a minimal $\mathbb{Z}$-generator of $\tau(\mathcal{G})$ if and only if it satisfies one of the following conditions*

(i) ω has degree 1 and ω is a network, or

(ii) ω has degree 2, and satisfies the following three conditions determining w_0

$e^*(\omega) = 1$, *for all cycle edges $e \in \mathcal{E} \setminus \mathcal{L}$*

$e^*(\omega) = 2$, *for an odd number of cycle legs,*

$e^*(\omega) = 0$, *for the remaining cycle legs.*

Each of the remaining components $\omega_i \in \tau(\mathcal{G}_i)$ is an element of degree at most two.

We postpone the proof until we prepare for it with some lemmas. The idea of the proof is to use Lemma II.32 in order to remove the pendant trees $\mathcal{G}_1, \ldots, \mathcal{G}_k$ and work only with the polygon graph $\mathcal{G}_0$. Lemma II.41 describes all the degree 2 points of the cone of a polygon graph and distinguishes the generators among them.

Example II.38. In Figure II.10 we illustrate the generators of the cone associated to the graph LittleMan (one of the two graphs with one cycle and two leaves). The first four are of degree 1, the remaining three are of degree 2.

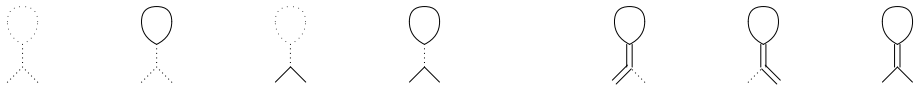


Fig. II.10.: Generators of the cone of the LittleMan graph

Lemma II.39 (Decomposition propagates to pendant trees)**.** *Let $\mathcal{G}$ be any trivalent graph and $\omega \in \tau$ any cone element. Let us also fix a non-cycle edge $e \in \mathcal{E} \setminus \mathcal{P}$ such that $\mathcal{G}^e$ is a tree, where $\mathcal{G}^e = \mathcal{G}_1 \sqcup \mathcal{G}_2$. Then any decomposition of $\rho_1^e(\omega)$ lifts to a decomposition of ω.*

Proof. First note that both ρ_1^e and ρ_2^e preserve the degree, so an element ω of degree d in $\tau(\mathcal{G})$ yields $\omega_1 \in \tau(\mathcal{G}_1)$ and $\omega_2 \in \tau(\mathcal{G}_2)$ both of degree d. The semigroup of a tree is generated by networks, which are degree 1 elements, see Theorem II.36. This means that $\rho_2^e(\omega)$ is a sum of degree 1 elements. Thus if $\rho_1^e(\omega)$ can be decomposed, then the same decomposition works for ω by choosing appropriate grouping of the summands of $\rho_2^e(\omega)$, because the degrees are preserved. □

Corollary II.40. *In the proof of Theorem II.37 we can assume that the graph is a polygon graph.*

Proof. A graph with one cycle is a polygon graph with a tree attached to each cycle leg $l_1, \ldots, l_k$. We cut all the cycle legs to obtain $k+1$ pieces of the graph $\mathcal{G}$: a polygon graph $\mathcal{G}_0$ and k trees: $\mathcal{G}_1, \ldots, \mathcal{G}_k$. We denote by ρ_0 the composition of projections for each leg that we cut $\rho_0 = \rho_0^{l_1} \circ \cdots \circ \rho_0^{l_k}$. Iteratively using Lemma II.39 to decompose $\rho_0(\omega)$ we decompose ω. □

Lemma II.41 (Degree 2 elements of the cone)**.** *Let $\mathcal{G}$ be a graph with exactly one cycle. Any degree 2 element of $\tau(\mathcal{G})$ except those in Theorem II.37 (ii) is a sum of two networks.*

Proof. By Corollary II.40 we may assume $\mathcal{G}$ is a polygon graph. Let $\omega \in \tau(\mathcal{G})$ a degree 2 element. The coefficient $e^*(\omega)$ of ω on any edge $e \in \mathcal{E}$ is $0, 1$ or 2. We denote by

$$\omega_{\mathcal{E}\setminus\mathcal{P}} := \{e^*(\omega) \mid e \in \mathcal{E} \setminus \mathcal{P}\}$$

the set of coefficients of ω on the cycle edges. We distinguish between four types of ω based on $\omega_{\mathcal{E}\setminus\mathcal{P}}$. For all but one we decompose ω as a sum of two networks.

If $0 \in \omega_{\mathcal{E}\setminus\mathcal{P}}$, there exists a cycle edge $e \in \mathcal{E}(\mathcal{G})$ with $e^*(\omega) = 0$. We can cut it with no harm to ω, since $i^e(\omega) \in \tau(\mathcal{G}^e)$ is a degree 2 element in a cone of the trivalent tree $\mathcal{G}^e$, so it can be decomposed into a sum of degree 1 elements. This decomposition can be lifted to $\tau(\mathcal{G})$, as we assumed $e^*(\omega) = 0$. On Figure II.11 we show an example of this situation.

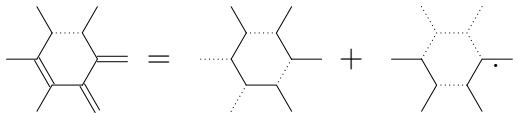


Fig. II.11.: Decomposition of a degree two element with a weight zero cycle edge

The second case is when $\omega_{\mathcal{E}\setminus\mathcal{P}} = \{2\}$, that is $e^*(\omega)$ is 2 on all cycle edges. As ω has degree 2, we know that $\deg_v(\omega) \leq 2$ and as a consequence:

$$e^*(\omega) = \begin{cases} 2 & \text{if } e \text{ is a cycle edge} \\ 0 & \text{otherwise, i.e. } e \text{ is a cycle leg.} \end{cases}$$

Thus ω is twice the network consisting of all the cycle edges, as on the example on Figure II.12.

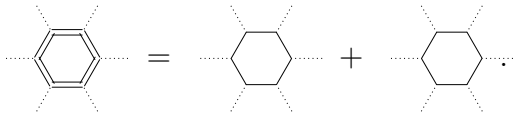


Fig. II.12.: Decomposition of a degree two element with all cycle edges of weight two

For the last two cases we let $l_1, \ldots, l_p$ be the set of all cycle legs with $l_i^*(\omega) \neq 0$ ordered anticlockwise and indexed by elements of $\mathbb{Z}_p$. Also we denote by $i \curvearrowleft j$ the path that starts at l_i and goes anticlockwise along the intermediate cycle edges to l_j and ends there.

In the third case $\omega_{\mathcal{E}\setminus\mathcal{P}} = \{1\}$ and we will show that ω can be decomposed into a sum of two networks if and only if the number of cycle legs for which ω has a coefficient 2 is even. Suppose we have decomposed $\omega = \omega_1 + \omega_2$ into a sum of networks and neither ω_1 nor ω_2 contains the path consisting of all cycle edges (in which case the other one would be an empty network). Then both ω_1 and ω_2 contain a positive even number of legs. Any path in ω_1 (respectively ω_2) is of the type $i \curvearrowleft i+1$, from the cycle leg l_i to the next one. If the end was not the next one, there would be a path in ω_2 (respectively ω_1) containing an intermediate leg and as a result there would be a cycle edge e with $\omega(e) = 2$, but $\omega_{\mathcal{E}\setminus\mathcal{P}} = \{1\}$. Moreover, both ω_1 and ω_2 contain all non-zero cycle legs, each with value 1, because they are both of degree 1 and in the cone we have $\deg(\omega) \geq \deg_{\min}(\omega)$. This is only possible when the number p of non-zero cycle legs is even, and in that case we have the obvious decomposition with $\omega_1 = \; i_1 \curvearrowleft i_2 \; + \; \ldots \; + \; i_{p-1} \curvearrowleft i_p$ and $\omega_2 = \; i_2 \curvearrowleft i_3 \; + \; \ldots \; + \; i_p \curvearrowleft i_1$. Otherwise ω is a generator. Examples of both these situations are drawn on Figure II.13.

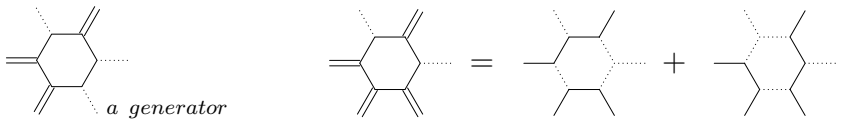


Fig. II.13.: Typical generator of degree two and a decomposition of a degree two element with all cycle edges of weight one

In the last case $\omega_{\mathcal{E}\setminus\mathcal{P}} = \{1, 2\}$. When $l^*(\omega) = 2$ we call l a two-leg. Denote by $l_{i_1}, \ldots, l_{i_q}$ the subsequence of two-legs, numbered in such way that traveling along the cycle anticlockwise from l_{i_q} to l_{i_1} there is a one-leg, provided that ω has some one-legs. We observe that the number of one-legs between two consecutive two-legs is always even. This is best explained by drawing the picture from Figure II.14.

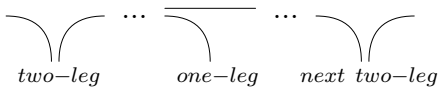


Fig. II.14.: Element of degree two has even number of one-legs between consecutive two-legs

where the arcs are our x_v, y_v, z_v's introduced in II.9. To produce an element of the lattice, the two on the same edge need to share the same value. If there would be only zero-legs where the first dots are, the local paths would not agree on some cycle edge.

The decomposition $\omega = (1, \omega_1) + (1, \omega_2)$ depends on the parity of q, which is the number of two-legs. We first work in the case $q = 2r$ is even, the odd case uses the same idea with small modifications. The Figure II.15 visualizes how the decomposition is constructed in the case $q = 4$.

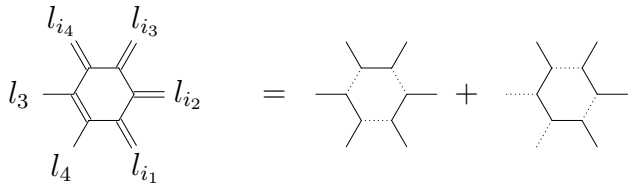


Fig. II.15.: Decomposition of a degree two element with even number of two-legs

First we place all paths between two consecutive two-legs starting at an leg with an even (respectively odd) index into ω_1 (respectively ω_2). Then, to take care of the one-legs, we add paths between consecutive one-legs lying between $l_{i_{2j}}$ and $l_{i_{2j+1}}$ for some $j \in \{1, \ldots, p\}$ to ω_1. Thus we get

$$\omega_1 = \begin{array}{llllll} i_1 \curvearrowleft i_2 & + & (i_2+1) \curvearrowleft (i_2+2) & +\ldots+ & (i_3-2) \curvearrowleft (i_3-1) & + \\ i_3 \curvearrowleft i_4 & + & (i_4+1) \curvearrowleft (i_4+2) & +\ldots+ & (i_5-2) \curvearrowleft (i_5-1) & + \\ & & \vdots & & & \\ i_{2r-1} \curvearrowleft i_{2r} & + & (i_{2r}+1) \curvearrowleft (i_{2r}+2) & +\ldots+ & (i_1-2) \curvearrowleft (i_1-1) & \end{array} .$$

Similarly we add paths between consecutive one-legs lying between $l_{i_{2j-1}}$ and $l_{i_{2j}}$ for some $j \in \{1, \ldots, p\}$ to ω_2. So we can write

$$\omega_2 = \begin{array}{llllll} i_2 \curvearrowleft i_3 & + & (i_3+1) \curvearrowleft (i_3+2) & +\ldots+ & (i_4-2) \curvearrowleft (i_4-1) & + \\ i_4 \curvearrowleft i_5 & + & (i_5+1) \curvearrowleft (i_5+2) & +\ldots+ & (i_6-2) \curvearrowleft (i_6-1) & + \\ & & \vdots & & & \\ i_{2r} \curvearrowleft i_1 & + & (i_1+1) \curvearrowleft (i_1+2) & +\ldots+ & (i_2-2) \curvearrowleft (i_2-1) & \end{array} .$$

Clearly those paths in ω_1 (resp. ω_2) are disjoint, so both are networks and by construction they yield a decomposition of our ω.

When the number q of two-legs is odd we need to adjust the above decomposition. Again, we draw an example on Figure II.16 for $q = 3$

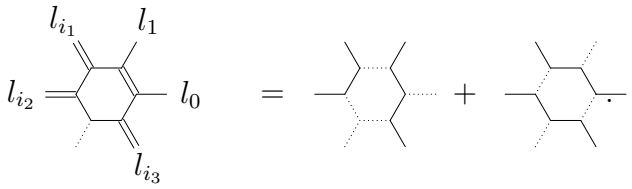


Fig. II.16.: Decomposition of a degree two element with odd number of two-legs

As there is an odd number of two-legs, we will use two consecutive one-legs lying between l_{i_q} and l_{i_1} to make up for the missing two-leg, and we proceed as before to get

$$\omega_1 = \begin{array}{ll} i_1 \curvearrowleft i_2 & + \quad (i_2+1) \curvearrowleft (i_2+2) + \ldots + (i_3-2) \curvearrowleft (i_3-1) + \\ i_3 \curvearrowleft i_4 & + \quad (i_4+1) \curvearrowleft (i_4+2) + \ldots + (i_5-2) \curvearrowleft (i_5-1) + \\ & \vdots \\ i_{2r-1} \curvearrowleft i_{2r} & + \quad (i_{2r}+1) \curvearrowleft (i_{2r}+2) + \ldots + (i_{2r+1}-2) \curvearrowleft (i_{2r+1}-1) \\ i_{2r+1} \curvearrowleft i_1 - 1 & \end{array}$$

and

$$\omega_2 = \begin{array}{ll} i_2 \curvearrowleft i_3 & + \quad (i_3+1) \curvearrowleft (i_3+2) + \ldots + (i_4-2) \curvearrowleft (i_4-1) + \\ i_4 \curvearrowleft i_5 & + \quad (i_5+1) \curvearrowleft (i_5+2) + \ldots + (i_6-2) \curvearrowleft (i_6-1) + \\ & \vdots \\ i_{2r} \curvearrowleft i_{2r+1} & + \quad (i_{2r+1}+1) \curvearrowleft (i_{2r+1}+2) + \ldots + (i_1-4) \curvearrowleft (i_1-3) \\ i_1 - 2 \curvearrowleft i_1 & \end{array}$$

This ends the proof of the lemma about the decomposable degree two elements of the cone. □

Proof of Theorem II.37. The proof yields an algorithm for decomposing an arbitrary element ω of the cone $\tau(\mathcal{G})$ into a sum of degree 1 and 2 generators. By Corollary II.40 we only need to prove the theorem when $\mathcal{G}$ is a polygon graph. First we fix an orientation of the cycle of $\mathcal{G}$ and we call it anticlockwise in order to think of a planar embedding of the graph. Let $\omega \in \tau(\mathcal{G})$. We will find an element μ of degree at most 2, such that $\omega - \mu \in \tau(\mathcal{G})$. Let v be a vertex and l_v the cycle leg attached it. We choose an map $i_v : \curlywedge \to \mathcal{G}$ so that the edge e_3 is mapped to l_v, the edge e_2 is mapped to the edge which points anticlockwise from v, and the edge e_1 is mapped to the edge which points clockwise from v. In this notation the coefficient of ω at l_v

is measured by c_v and coefficient of the edge anticlockwise (respectively clockwise) from v is measured by a_v (respectively b_v). We will also use the local paths x_v, y_v, z_v defined in (II.9).

Now we are ready to describe the algorithm to find μ.

Step 1. If there is a cycle edge e with $e^*(\omega) = 0$, we cut e and obtain the graph $\mathcal{G}^e$ which is a trivalent tree. Thus $\rho^e(\omega)$ is a sum of networks of path and this decomposition lifts to graph $\mathcal{G}$.

Step 2. Otherwise $e^*(\omega) \geq 1$ on all cycle edges e. We set μ to have value 1 on every cycle edge. Equivalently μ is defined by setting at every cycle vertex $z_v(\mu) = 1$, $x_v(\mu) = 0$, $y_v(\mu) = 0$. Now if $\omega - \mu \in \tau(\mathcal{G})$ we are done. Otherwise $\omega - \mu$ fails one of the inequalities defining $\tau(\mathcal{G})$. It is not the one with degrees, since for each vertex $v \in \mathcal{G}$ we have $\deg_v(\mu) = 1$, which implies $\deg_{\min}(\omega - \mu) \leq \deg(\omega) - \deg(\mu) = \deg(\omega - \mu)$. Clearly all coefficients of $\omega - \mu$ are positive. Thus at some vertex $v \in \mathcal{V}$ our $\omega - \mu$ fails one of the triangle inequalities.

Step 3. We will adjust μ to fix the triangle inequalities for $\omega - \mu$. If a triangle inequality for $\omega - \mu$ at v fails, then this is because $z_v(\omega) = 0$. In such a case we set $\mu(l_v) = 2$, which will not make any coefficient of $\omega - \mu$ negative provided $c_v(\omega) \geq 2$. But since $a_v(\omega), b_v(\omega) \geq 1$ and $z_v(\omega) = 0$ we must have $x_v(\omega), y_v(\omega) \geq 1$. This implies $c_v(\omega) \geq 2$ as required. In terms of x_v, y_v, z_v we have decreased $z_v(\mu)$ by one and increased both $x_v(\mu)$ and $y_v(\mu)$ by one.

Step 4. We need a last adjustment on μ to assure the additivity of degree where it is attained, i.e. for any v such that $\deg_v(\omega) = \deg(\omega)$ we need $\deg_v(\mu) = 2$ since $\deg(\mu) = 2$. This is to ensure $\omega - \mu \in \tau$. We call v *degree deficient vertex* if $\deg_v(\omega) = \deg(\omega)$ and $\deg_v(\mu) = 1$.

If v is degree deficient and in addition $x_v(\omega) > 0$ and $y_v(\omega) > 0$ we set $x_v(\mu) = y_v(\mu) = 1$ and $z_v(\mu) = 0$.

If v is degree deficient and both $x_v(\omega) = y_v(\omega) = 0$ are zero, then $z_v(\omega) = \deg_v(\omega)$, so at both next and previous cycle vertex the degree is attained

$$\deg_{v_{next}}(\omega) = \deg_{v_{prev}}(\omega) = \deg(\omega)$$
$$\text{since} \qquad z_{v_{next}} + y_{v_{next}} = z_v + x_v = z_{v_{prev}} + x_{v_{prev}} \tag{II.42}$$

If all degree deficient vertices were of this type, then ω was a multiple of the path consisting of all cycle edges.

Now we divide the set of all deficient vertices (which all have at least one of $x_v(\omega)$ or $y_v(\omega)$ equal to zero) into sequences of adjacent ones. Let us fix our attention to such a sequence (we already excluded the case when it has the same end and beginning). Call it $v_1, \ldots, v_r$. Then because all v_i's are degree deficient: $\deg(\omega) = \deg_{v_i}(\omega)$. The last one has $y_{v_r}(\omega) > 0$ by (II.42)

$$\deg(\omega) = z_{v_{r-1}}(\omega) = y_{v_r}(\omega) + z_{v_r}(\omega) \leq z_{v_r}(\omega) < \deg(\omega)$$

In the same way $x_{v_1}(\omega) > 0$. Finally all the middle ones have $z_{v_i}(\omega) > 1$. This implies that we can redefine μ on our fixed sequence $v_1, \ldots, v_r$ preserving all other properties and fixing the degree deficiency:

$$\begin{array}{lll} x_{v_1}(\mu) = 1 & x_{v_i}(\mu) = 0 & x_{v_r}(\mu) = 0 \\ y_{v_1}(\mu) = 0 & y_{v_i}(\mu) = 0 & y_{v_r}(\mu) = 1 \\ z_{v_1}(\mu) = 1 & z_{v_i}(\mu) = 2 & z_{v_r}(\mu) = 1 \end{array}$$

where $i \in \{2, \ldots, r-1\}$. We do this for all such sequences and we have the

required μ.

Now μ is an element of degree 2 and is either a generator or can be decomposed into a sum of two generators in degree 1, as described in Lemma II.41. □

Remark II.43. If we allow more cycles, we can have generators of higher degree. As we can see on Figure II.17 the graph with two loops and one leaf has a degree three generator: one on the two loops, two on the three other edges.

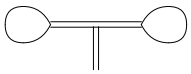


Fig. II.17.: Example of a degree three generator

3.4. Embedding

The aim of this section is to find a common ambient space for phylogenetic models of all graphs with the same topological invariants. The way to construct this ambient space follows easily form the definition of the model.

Theorem II.44. *The phylogenetic model of a trivalent graph $\mathcal{G}$ embeds in a projective toric variety $\mathbb{P}_{g,n}$, which is a good quotient of projective space by an action of a g-dimensional torus. This action as well as the variety $\mathbb{P}_{g,n}$ depends only on the first Betti number and number of leaves of $\mathcal{G}$, up to reordering of coordinates.*

Proof. Models of trivalent trees with N leaves embed naturally in $\mathbb{P}^{2^{N-1}-1}$, with coordinates x_κ where $\kappa \in \{0,1\}^N$ is a sequence of length N with values in $\{0,1\}$ and even number of 1-entries, see Proposition II.36. We cut g cycle edges of the graph $\mathcal{G}$ so that we obtain a trivalent tree $\mathcal{T}$ with set S of $M = n + 2g$ leaves. Dividing

$\mathbb{P}^{2^{M-1}-1}$ by the action of the g-dimensional torus $\mathbb{T}(g,n)$ that corresponds to gluing these leaves back together, yields the required embeddings.

We will now explain that this action does not depend on the graph $\mathcal{G}$, up to choice of coordinates on Let us label the set of leaves by $1 \dots M$ and divide it into three disjoint sets $S = S_0 \sqcup S_1 \sqcup S_{-1}$ as follows. S_0 is the set of leaves of the original graph $\mathcal{G}$. The $2g$ new leaves of $\mathcal{T}$ come in pairs (l, l^-), where both l and l^- used to be the same edge in $\mathcal{G}$. We put l in S_1 and l^- in S_{-1}.

The action of the g-dimensional torus $\mathbb{T}(g,n)$ on $\mathbb{P}^{2^{M-1}-1}$ is given by a matrix

$$\{\zeta_\kappa^l\}_{\kappa\in\{0,1\}^M}^{l=1\dots g} \text{ , where } \quad \zeta_\kappa^l = \kappa_l - \kappa_{l^-}$$

Thus this action is independent of the shape of $\mathcal{G}$ and depends only on (g,n) up to choice of order of coordinates. □

We will now illustrate Theorem II.44.

Example II.45. We describe $X\,(\text{♀})$, the model of LittleMan, together with its embedding into $\mathbb{P}_{1,2}$. We know that the model of a trivalent tree $\curlyvee$ is a complete intersection of two quadrics, see [5, Ex. 2.6],

$$(x_{1100}x_{0011} - x_{0000}x_{1111}, \quad x_{1001}x_{0110} - x_{1010}x_{0101}) \\ \subset \operatorname{Proj}\mathbb{C}[x_{0000}, x_{1100}, x_{0011}, x_{1111}, x_{1010}, x_{1001}, x_{0101}, x_{0110}] \quad \text{(II.46)}$$

where each variable x_κ corresponds to a degree 1 generator $\tau(\curlyvee)$. By Proposition II.36 a generator is given by its values on the leaves, which form the index $\kappa \in \{0,1\}^4$.

To obtain $X\,(\text{♀})$, we glue two leaves, say leaf e_1 is glued with the leaf e_2 to get the loop in LittleMan as shown on Figure II.18.

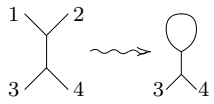


Fig. II.18.: Obtaining LittleMan graph from a four-leaf tree

Now $X\,(\text{\Large\textkeystroke})$ is a GIT-quotient of $X\,(\text{\Large\textkeystroke})$ by the action $\lambda^{e_1-e_2}$.

In the same way it embeds in a GIT-quotient of $\mathbb{P}^7$. One easily sees that

$$\mathbb{P}^7/\!\!/\mathbb{C}^* = V(y_1 \cdot y_2 - z_1 \cdot z_2) \subset \mathbb{P}(1^4, 2^4)$$

where

$$\mathbb{P}(1^4, 2^4) = \operatorname{Proj} \mathbb{C}[x_{0000}, x_{1100}, x_{0011}, x_{1111}, y_1, y_2, z_1, z_2]$$

is a weighted projective space and

$$y_1 = x_{1001} \cdot x_{0110}, \quad y_2 = x_{1010} \cdot x_{0101}, \quad z_1 = x_{1010} \cdot x_{0110}, \quad z_2 = x_{0101} \cdot x_{1001}$$

are the $\mathbb{C}^*$–invariant variables of degree 2. From Theorem I.6 it follows that $X\,(\text{\Large\textkeystroke})$ is given by Equations (II.46) of $X\,(\text{\Large\textkeystroke})$ in $\mathbb{P}^7$, rewritten in the coordinates of $\mathbb{P}^7/\!\!/\mathbb{C}^*$. The second one becomes $y_1 - y_2 = 0$, so

$$\begin{array}{ccccccc}
X\,(\text{\Large\textkeystroke}) & = & \operatorname{Proj} \mathbb{C}[\tau\,(\text{\Large\textkeystroke})] & = & V(x_{1100}x_{0011} - x_{0000}x_{1111}, y_1^2 - z_1 z_2) & \subset & \mathbb{P}(1^4, 2^3) \\
 & & & & & & \| \\
 & & \bigcap & & & & V(y_1 - y_2) \\
 & & & & & & \bigcap \\
\mathbb{P}_{1,2} & = & \mathbb{P}^7/\!\!/\mathbb{C}^* & = & V(y_1 y_2 - z_1 z_2) & \subset & \mathbb{P}(1^4, 2^4)
\end{array}$$

If we replace each variable in the equations of $X(\text{\Large\textkeystroke})$ by its representation on the graph, we get the picture from Figure II.19.

Fig. II.19.: Ideal of the model LittleMan graph

Example II.47. As in the previous example, we work out properties of $X\,(\text{-}\diamond\text{-})$ — the model of Hammock. We use the same action $\lambda^{l_1-l_2}$, but we change the embedding $X\,(\bowtie) \hookrightarrow \mathbb{P}^7$ by relabeling the leaves as on Figure II.20.

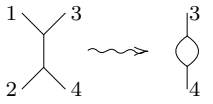


Fig. II.20.: Obtaining Hammock graph from a four-leaf tree

As the labeling of $\bowtie$ was modified, Equations (II.46) become

$$V(x_{1010}x_{0101} - x_{0000}x_{1111}, \quad x_{1001}x_{0110} - x_{1100}x_{0011}) \subset \mathbb{P}^7.$$

We again rewrite them in the invariant coordinates of $\mathbb{P}(1^4, 2^4)$ to get:

$$\begin{array}{ccccccc} X\,(\text{-}\diamond\text{-}) & = & \operatorname{Proj}\mathbb{C}[\tau\,(\text{-}\diamond\text{-})] & = & V(x_{0000}x_{1111}x_{1100}x_{0011} - z_1z_2) & \subset & \mathbb{P}(1^4, 2^2) \\ & & & & & & \| \\ & & \bigcap & & V(y_1 - x_{0000}x_{1111}, x_{1100}x_{0011} - y_2) & & \\ & & & & & & \bigcap \\ \mathbb{P}_{1,2} & = & \mathbb{P}^7/\!\!/\mathbb{C}^* & = & V(y_1y_2 - z_1z_2) & \subset & \mathbb{P}(1^4, 2^4) \end{array}$$

If we replace each variable in the degree 4 equation of $X(\text{-}\diamond\text{-})$ by its representation on the graph, we get the picture shown on Figure II.21.

Fig. II.21.: Ideal of the model of the Hammock graph

CHAPTER III

FLAT FAMILIES

Like in many branches of mathematics, algebraic geometry aims often to classify the objects of its study. One common restriction is to look only at (Zariski) closed subvarieties of a fixed projective space. A variety of this type is called *projective*. The class of projective varieties is a subclass of complete varieties, which are analogous to the compact spaces in topology.

There are number of ways to classify algebraic varieties. The easiest is to define discrete invariants, for example dimension or degree of a subvariety in a projective space. All the discrete invariants are captured by the *Hilbert polynomial*.

Another way of determining how similar varieties are is to ask if they can be deformed one to another by arranging a flat family with a connected base which contains both of them. If this can be done, they are called *deformation equivalent*.

The most important property of the Hilbert polynomial is exhibited by the following theorem.

Theorem. *Two subvarieties of a given projective space are deformation equivalent if and only if they have the same Hilbert polynomial.*

Another central fact of projective algebraic geometry says that there exists an object called *Hilbert scheme* parametrizing all projective varieties with a common ambient space. In 1966 Robin Hartshorne in his PhD thesis [12] proved that the connected components of the Hilbert scheme are in one-to-one correspondence with the set of possible Hilbert polynomials.

Models of trivalent trees that differ by one mutation live in a flat family in a projective space [5]. This statement almost remains true for trivalent graphs, by the

same argument. The only difference is that we get a family in the projective toric variety $\mathbb{P}_{g,n}$ instead of a usual projective space.

Recall that in Remark II.20 we have associated to a subset of leaves $\mathcal{S} \subset \mathcal{L}$ with k elements an action of a k-dimensional torus $\mathbb{T}(\mathcal{S})$ on the model $X(\mathcal{G})$.

1. Key examples of flat families for graph models

We construct two-dimensional flat families containing models of small graphs. They become the building blocks for deformations of bigger graphs.

Example III.1 (g=0, n=4)**.** Let $\curlyvee$ be a trivalent tree with four leaves. In [5, Ex. 2.20] we constructed a flat family

$$\mathcal{X}^0 \hookrightarrow \mathcal{B} \times \mathbb{P}^7,$$

where

- $\mathcal{B}$ is an open subset of $\mathbb{P}^2$ with coordinates $b_{(1,2)(3,4)}$, $b_{(1,3)(2,4)}$, $b_{(1,4)(2,3)}$
- the torus $\mathbb{T}(\mathcal{L})$ acts on $\mathcal{B} \times \mathbb{P}^7$ via the second coordinate, that is, for a leaf l of $\curlyvee$ and coordinate x_κ of $\mathbb{P}^7$ we have $\lambda_{v_i}(t)(b_{(.)(.)}, x_\kappa) = (b_{(.)(.)}, t^{\kappa(l)} x_\kappa)$,
- the equidimentional projection $\mathcal{X}^0 \to \mathcal{B}$ contains the three special fibers $\mathcal{X}^0_{[1,0,0]}$, $\mathcal{X}^0_{[0,1,0]}$ and $\mathcal{X}^0_{[0,0,1]}$ which are models of aforementioned four-leaf trees,
- $\mathcal{X}^0$ is a $\mathbb{T}(\mathcal{L})$-invariant complete intersection in $\mathcal{B} \times \mathbb{P}^7$ of the two quadrics

$$b_{(12)(34)} \cdot x_{1100}x_{0011} \; + \; b_{(13)(24)} \cdot x_{1010}x_{0101} \; + \; b_{(14)(23)} \cdot x_{1001}x_{0110}$$
$$- \; \big(b_{(12)(34)} + b_{(13)(24)} + b_{(14)(23)}\big) \cdot x_{0000}x_{1111}$$

$$\big(b_{(13)(24)} - b_{(14)(23)}\big) \cdot x_{1100}x_{0011} + \big(b_{(14)(23)} - b_{(12)(34)}\big) \cdot x_{1010}x_{0101}$$
$$+ \big(b_{(12)(34)} - b_{(13)(24)}\big) \cdot x_{1001}x_{0110}.$$

Example III.2 ($g = 1$, $n = 2$)**.** We construct a family which contains models of graphs with one cycle and two leaves. It arises as a $\mathbb{C}^*$-quotient of the family $\mathcal{X}^0 \hookrightarrow \mathbb{P}^7$ from Example III.1. Let us fix a $\mathbb{C}^*$-action $\lambda^{l_1-l_2}$ on the ambient $\mathbb{P}^7$, thus on $\mathcal{X}^0$ and tree models as well, by choosing leaves l_1 and l_2 labeled by 1 and 2 respectively. Each of the three trees yields a graph, when two leaves are glued together. Up to graph isomorphism, there are two graphs with one cycle and two leaves. As we are mutating along fixed edge, the LittleMan appears once and the Hammock twice. The picture of the three possible trees becomes the one on Figure III.1.

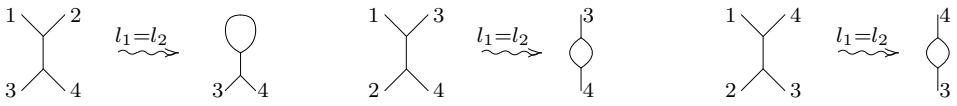


Fig. III.1.: Mutations of graphs with one cycle and two leaves

The new ambient space $\mathbb{P}^7/\!\!/\mathbb{C}^* = (y_1 \cdot y_2 - z_1 \cdot z_2) \subset \mathbb{P}(1^4, 2^4)$ was discussed in Example II.45.

By Theorem I.6, the new family $\mathcal{X}^0/\!\!/\mathbb{C}^*$ is given by the same, $\mathbb{T}(S)$-invariant

equations of $\mathcal{X}^0$. We rewrite them in the (invariant) coordinates of $\mathbb{P}(1^4, 2^4)$

$$b_{(12)(34)} \cdot x_{1100}x_{0011} + b_{(13)(24)} \cdot y_2 + b_{(14)(23)} \cdot y_1 - (b_{(12)(23)} + b_{(13)(24)} + b_{(14)(23)}) \cdot x_{0000}x_{1111},$$

$$(b_{(23)(14)} - b_{(14)(23)}) \cdot x_{1100}x_{0011} + (b_{(14)(23)} - b_{(12)(34)}) \cdot y_2 + (b_{(12)(34)} - b_{(23)(14)}) \cdot y_1,$$

$$y_1 \cdot y_2 - z_1 \cdot z_2.$$

To understand how this works a little better, let us look at particular coordinate of $\mathbb{P}(1^4, 2^4)$, say $y_2 = x_{1001}x_{0110}$, and draw on Figure III.2 its representation for each graph.

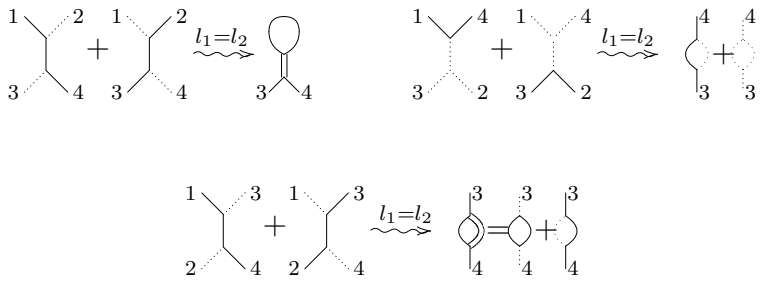


Fig. III.2.: Behavior of coordinates of $\mathbb{P}_{1,2}$ under mutations

2. Deformation equivalent models

We construct a flat family containing models of all mutations of a given trivalent graph $\mathcal{G}$ along a fixed edge $e \in \mathcal{E} \setminus \mathcal{P}$. We follow [5, Const. 3.5] replacing polytopes by cones.

Let $\mathcal{G}$ be a graph with an inner edge e_0 which contains two trivalent inner vertices. We can write $\mathcal{G}$ as a sum of a not necessarily connected graph $\mathcal{G}_1$ with a set S of k distinguished leaves $l_1, \ldots, l_k$ with $k \in \{0, \ldots, 4\}$ and a graph $\mathcal{G}_0$ having the edge e_0

as its inner edge and $\mathcal{G}_0$ is one of the following three small graphs

(i) a tree  with four leaves $v_1, \ldots, v_4$, where the edge incident to the leaf l_i is identified with the edge incident to the leaf v_i,

(ii) LittleMan or Hammock  — a graph with four edges and two leaves v_1 and v_2,

(iii) Dumbell a graph with three edges and two loops and no leaves.

From Proposition II.29 we can compute the lattice $M^{gr}(\mathcal{G})$ and the cone $\tau(\mathcal{G})$ from those of the pieces $\mathcal{G}_0$ and $\mathcal{G}_1$

$$M^{gr}(\mathcal{G}) = M^{gr}(\mathcal{G}_0) \times_g M^{gr}(\mathcal{G}_1) \cap \bigcap_{i=1}^{k} \ker(\ell_i - v_i)$$
$$\tau(\mathcal{G}) = \tau(\mathcal{G}_0) \times_g \tau(\mathcal{G}_1) \cap \bigcap_{i=1}^{k} \ker(\ell_i - v_i).$$

We consider the lattice M^{gr}_{amb} and the cone τ_{amb}, which are the combinatorial data of the ambient space $\mathbb{P}_{g(\mathcal{G}_0),n(\mathcal{G}_0)}$ described by Theorem II.44, Example II.45 and Example II.47. The inclusion $X(\mathcal{G}_0) \subset \mathbb{P}_{g(\mathcal{G}_0),n(\mathcal{G}_0)}$ yields maps: $M^{gr}_{amb} \to M^{gr}(\mathcal{G}_0)$ and $\tau_{amb} \to \tau(\mathcal{G}_0)$. Forms v_i, $i = 1, \ldots k$ pull-back to M^{gr}_{amb} and we denote them by $\tilde{v}_i$, respectively. Now we define

$$M^{gr}_{\mathcal{Y}} = M^{gr}_{amb}(\mathcal{G}_0) \times_g M^{gr}(\mathcal{G}_1) \cap \bigcap_{i=1}^{k} \ker(\ell_i - \tilde{v}_i)$$
$$\tau_{\mathcal{Y}} = \tau_{amb}(\mathcal{G}_0) \times_g \tau(\mathcal{G}_1) \cap \bigcap_{i=1}^{k} \ker(\ell_i - \tilde{v}_i).$$

We define a toric variety $\mathcal{Y} = \operatorname{Proj} \mathbb{C}[\tau_{\mathcal{Y}}]$. Since the good quotient is a categorical quotient, by the construction we have the embedding

$$X(\mathcal{G}) \hookrightarrow \mathcal{Y}.$$

Lemma III.3. *The inclusions*

$$M^{gr}_{\mathcal{Y}} \hookrightarrow M^{gr}_{amb} \times \ M^{gr}(\mathcal{G}_1) \quad \text{and} \quad \tau_{\mathcal{Y}} \hookrightarrow \tau_{amb} \times \tau(\mathcal{G}_1)$$

induce a rational map

$$\mathbb{P}_{g(\mathcal{G}_0),n(\mathcal{G}_0)} \times X(\mathcal{G}_1) \dashrightarrow \mathcal{Y}$$

which is a good quotient map (of the set over which it is defined) with respect to the action of the k-dimensional torus $\mathbb{T}_0$ generated by one-parameter groups $\lambda_{v_i - \ell_i}$, where $i = 1, \dots k$. The subvariety

$$\widehat{\mathcal{X}} = \mathcal{X}^0 \times X(\mathcal{G}_1) \hookrightarrow \mathcal{B} \times \mathbb{P}^7 \times X(\mathcal{G}_1)$$

is $\mathbb{T}_0$-invariant and its quotient $\mathcal{X}$ is locally complete intersection in $\mathcal{B} \times \mathcal{Y}$.

Proof. The map given by inclusions of cones and lattices is a good quotient map by Theorem I.14. Invariance of the resulting subvariety $\widehat{\mathcal{X}}$ follows by the invariance of $\mathcal{X}^0 \hookrightarrow \mathcal{B} \times \mathbb{P}^7$ discussed in Example III.1. Finally, since $\widehat{\mathcal{X}}$ is a complete intersection in $\mathcal{B} \times \mathbb{P}^7 \times X(\mathcal{G}_1)$ its image $\mathcal{X}$ is a locally complete intersection in the quotient $\mathcal{B} \times \mathcal{Y}$. This follows from the definition of good quotient, which locally is an affine quotient, [2, Ch. 5], hence functions defining $\widehat{\mathcal{X}}$ locally descend to functions defining $\mathcal{X}$. □

Lemma III.4. *Over an open set $\mathcal{B}' \subset \mathbb{P}^2$ containing points $[1,0,0]$, $[0,1,0]$, $[0,0,1]$ the projection morphism $\mathcal{X} \to \mathcal{B}'$ is flat. The fibers over points $[1,0,0]$, $[0,1,0]$, $[0,0,1]$ are reduced and isomorphic to, respectively, the geometric model of $\mathcal{G}$ and of its elementary mutations along the edge e_0.*

Proof. First we note that the fibers in question, $\mathcal{X}_{[*,*,*]}$, of $\mathcal{X} \to \mathcal{B}$ are geometric models as we claim. Indeed this follows from the universal properties of good quotients, c.f. [2], as they are quotients of the respective products $\mathcal{X}^0_{[*,*,*]} \times X(\mathcal{G}_1)$, which are located, as three invariant subvarieties, in $\widehat{\mathcal{X}} = \mathcal{X}^0 \times X(\mathcal{G}_1)$. This, in particular, implies that the respective fibers of $\mathcal{X} \to \mathcal{B}$ are of the expected dimension, hence they are contained in a set $\mathcal{B}' \subset \mathbb{P}^2$ over which the map in question is equidimentional. Since $\mathcal{Y}$ is toric it is Cohen-Macaulay and because $\mathcal{X}$ is a locally complete intersection in $\mathcal{Y}$, it is Cohen-Macaulay too [7, Prop. 18.13]. Finally, the map $\mathcal{X} \to \mathcal{B}'$ is equidimentional hence it is flat, because $\mathcal{B}'$ is smooth, see [7, Thm. 18.16] □

Theorem III.5. *Geometric models of connected trivalent graphs with the same number of leaves n and cycles g are deformation equivalent in the projective toric variety $\mathbb{P}_{g,n}$, which is a quotient of $\mathbb{P}^{2^{n+2g-1}-1}$ by a g-dimensional torus.*

Proof. This is a combination of Proposition II.11 and of Lemma III.4. □

Remark III.6. Since the phylogenetic model of disjoint union of graphs is a product of the models of the pieces, see II.29, we have proved that models of graphs with the same topological invariants are deformation equivalent.

CHAPTER IV

HILBERT FUNCTION OF THE PHYLOGENETIC MODEL

As we mentioned in Chapter III, given a projective variety embedded in a projective space we have Hilbert function coming from the grading of the coordinates ring, or equivalently from the action of the one-dimensional torus $\mathbb{C}^*$. If our projective variety is equipped with an action of a bigger torus it is natural (see [11]) to consider a *multigraded Hilbert function*, whose domain consists of the characters of the torus.

We study multigraded Hilbert function of an embedded projective toric variety with the multigrading given by a subtorus of the big torus. For the graph model $X(\mathcal{G})$ the subtorus comes from a subset of leaves. We prove in Theorem IV.5 that the Hilbert function depends only on the topological invariants of the graph by showing that deformations constructed in the proof of Theorem III.5 preserve the whole Hilbert series. As tools we use Lemma IV.3 to compute the Hilbert series of a torus invariant complete intersection. Lemma IV.4 gives the formula for the Hilbert series of a quotient of a toric variety by a subtorus of the big torus. We first state them in the algebraic setting.

1. Rings with torus actions

Let R be a commutative $\mathbb{C}$-algebra with an action of a torus $\mathbb{T}$. Let $M_{\mathbb{T}} = \{\chi : \mathbb{T} \to \mathbb{C}^*\}$ denote the group of characters of the torus $\mathbb{T}$. Then we can write

$$R = \bigoplus_{\chi \in M_{\mathbb{T}}} R_\chi$$

as a sum of isotypical pieces indexed by the characters of the torus. We assume that each R_χ has finite dimension over $\mathbb{C}$. Then its **Hilbert function** $H_{R,\mathbb{T}} : M_\mathbb{T} \to \mathbb{N}$ is

$$H_{R,\mathbb{T}}(\chi) := \dim R_\chi.$$

The **Hilbert series** is the generating series of $H_{R,\mathbb{T}}$

$$h_{R,\mathbb{T}}(t) := \sum_{\chi \in M_\mathbb{T}} \dim R_\chi \cdot t^\chi.$$

Lemma IV.1. *Let $R = \bigoplus_{\chi \in M_\mathbb{T}} R_\chi$ be a ring with a torus action. If $f_1, \ldots, f_q$ are homogeneous with $f_i \in R_{\chi_i}$ and form a regular sequence in R, then*

$$h_{R/\langle f_1,\ldots,f_q\rangle,\mathbb{T}}(t) = h_R(t) \cdot (1 - t^{\chi_1}) \cdot \ldots \cdot (1 - t^{\chi_q}).$$

Proof. The statement for the single graded Hilbert series is explicitly given in [22, Cor. 3.2]. Its multigraded, more general, with minor additional assumption can be found in [16, Claim 13.38]. The lemma follows by induction on the length of the regular sequence. For any homogenous $f \in R_{\chi_f}$ which is not a zero divisor in R and any $\chi \in M$ we have the exact sequence of $\mathbb{T}$-modules

$$0 \longrightarrow R_{\chi-\chi_f} \xrightarrow{f\cdot} R_\chi \longrightarrow (R/(f))_\chi \longrightarrow 0,$$

which implies that

$$H_{R/(f)}(\chi) = \dim (R/(f))_\chi = \dim R_\chi - \dim R_{\chi-\chi_f} = H_R(\chi) - H_R(\chi - \chi_f)$$

This is equivalent to the required equality for Hilbert series. □

Given a subtorus $\iota : \mathbb{S} \hookrightarrow \mathbb{T}$ we have the corresponding epimorphism of the character groups $\iota^* : M_\mathbb{T} \twoheadrightarrow M_\mathbb{S}$ and we can form the $\mathbb{S}$-invariant subring $R^\mathbb{S}$ of R

equipped with the residual action of the quotient torus $\mathbb{T}/\mathbb{S}$

$$R^{\mathbb{S}} = \bigoplus_{\chi \in M_{\mathbb{T}/\mathbb{S}}} R_\chi.$$

Then we have the following formula for the Hilbert series.

Lemma IV.2. *Let R be a ring equipped with an action of a torus $\mathbb{T}$ and let $\iota : \mathbb{S} \hookrightarrow \mathbb{T}$ be a subtorus. Then the Hilbert series of the invariant ring $R^{\mathbb{S}}$ is*

$$h_{R^{\mathbb{S}},\mathbb{T}/\mathbb{S}} = \sum_{\chi \in \ker \iota^*} t^\chi \dim R_\chi,$$

where $\iota^* : M_{\mathbb{T}} \twoheadrightarrow M_{\mathbb{S}}$ is the dual map of the character groups.

2. Toric variety with a distinguished subtorus

Let $X = \operatorname{Proj} R$ be a projective toric variety of dimension d with an ample Weil divisor $\mathcal{L}$ where $R = \bigoplus_{m\in\mathbb{N}} R_m = \bigoplus_{m\in\mathbb{N}} H^0(X, m\mathcal{L})$ as in Section 3. Then R has an action of a $d+1$ dimensional torus which is the product of the d-dimentional torus $\mathbb{T}$ of X and the $\mathbb{C}^*$ from the grading. Any subtorus $\mathbb{S} \hookrightarrow \mathbb{T}$ of dimension r induces a $\mathbb{Z}^{r+1}$-sub-grading. Then its **multigraded Hilbert function** $H_{X,\mathbb{S}} : M_{\mathbb{C}^*\times\mathbb{S}} \to \mathbb{N}$ **with respect to** $\mathbb{S}$ is

$$H_{X,\mathbb{S}}(\chi) := H_{R,\mathbb{S}}(\chi) = \dim R_\chi.$$

The generating series of $h_{R,\mathbb{S}}$ is the **multigraded Hilbert series with respect to** $\mathbb{S}$

$$h_{X,\mathbb{S}}(t) := h_R(t) = \sum_{\chi \in M_{\mathbb{S}}} \dim R_\chi \cdot t^\chi.$$

We have the following corollary of Lemma IV.1.

Corollary IV.3. *Let $Y = \operatorname{Proj} R$ be a projective toric variety with an action of an r-dimensional subtorus $\mathbb{S} \subset \mathbb{T}$ of the big torus. Let us assume that $X \subset Y$ is a*

$\mathbb{S}$-*invariant complete intersection in* Y *given by the ideal* $I(X) = \langle f_1, \ldots, f_q \rangle$, *where* $\deg f_i = \chi_i$. *Then the* $\mathbb{S}$-*graded Hilbert series of* X *is*

$$h_{X,\mathbb{S}}(t) = h_Y(t) \cdot (1 - t^{\chi_1}) \cdot \ldots \cdot (1 - t^{\chi_q}).$$

The next statement is a corollary of Lemma IV.2 by using the description of the quotient as the spectrum of invariants given in Theorem I.6.

Lemma IV.4. *Let* $X = \operatorname{Proj} R$ *be a projective toric variety with a subtorus* $\iota : \mathbb{S} \hookrightarrow \mathbb{T}$ *of the big torus as before. We assume that both actions are linearized with respect to the ample Weil divisor* $\mathcal{L}$. *Let* $\iota^* : M_{\mathbb{T}} \twoheadrightarrow M_{\mathbb{S}}$ *be the correspoding surjection of character lattices. Then*

$$h_{X/\!\!/\mathbb{S}}(t_0, t_1, \ldots, t_r) = \sum_{\chi \in \tau(X) \cap \ker \iota^*} t^{\chi} \cdot \dim R_{\chi}.$$

We combine the above facts to get the equality of the Hilbert series of models of mutation equivalent graphs.

Theorem IV.5. *Let* $\mathcal{G}_1$ *and* $\mathcal{G}_2$ *be mutation-equivalent graphs and* S_1 *(respectively* $\mathcal{S}_2$*) be a subset of leaves of* $\mathcal{G}_1$ *(respectively* $\mathcal{S}_2$*). Assume that* $|\mathcal{S}_1| = |\mathcal{S}_2|$. *Then the multigraded series with respect to the tori associated to those sets of leaves are equal*

$$h_{X(\mathcal{G}_1),\mathbb{T}(\mathcal{S}_1)} = h_{X(\mathcal{G}_2),\mathbb{T}(\mathcal{S}_2)}$$

Proof. Since they are mutation-equivalent by Lemma II.11 we can assume the sequence of mutation takes the set $\mathcal{S}_1$ to the set $\mathcal{S}_2$. We can assume $\mathcal{G}_1$ and $\mathcal{G}_2$ differ by one mutation. In Section III.2 we have constructed a flat family which is a complete intersection having the models $X(\mathcal{G}_1)$ and $X(\mathcal{G}_2)$ as fibers. Because both those models are complete intersections of the same type in the same ambient space by using Lemma IV.3 we conclude that the Hilbert series are equal. □

We illustrate Theorem IV.5 on examples.

Example IV.6. We compute the Hilbert series for the models of graphs with two leaves and the first Betti number one $X(\text{⚲})$ and $X(\text{-○-})$. As we saw in Example II.38 and in the notation of Example II.45, the cone $\tau(\text{⚲})$ has generators of the following multidegrees

coordinate	x_{0000}	x_{1100}	x_{0011}	x_{1111}	y_1	z_1	z_2
degree	$(1,0,0)$	$(1,0,0)$	$(1,1,1)$	$(1,1,1)$	$(2,1,1)$	$(2,2,0)$	$(2,0,2)$

and that $X(\text{⚲})$ is a complete intersection in $\mathbb{P}(1^4,2^3)$ of a quadric $x_{1100}x_{0011}-x_{0000}x_{1111}$ of multidegree $(2,1,1)$ and a quartic $y_1^2-z_1z_2$ of multidegree $(4,2,2)$. Thus

$$h_{X(\text{⚲}),\mathcal{L}(\text{⚲})}(t,s_1,s_2)=\frac{\cancel{(1-t^2s_1s_2)}\cdot(1-t^4s_1^2s_2^2)}{(1-t)^2\cdot(1-ts_1s_2)^2\cdot\cancel{(1-t^2s_1s_2)}\cdot(1-t^2s_1^2)\cdot(1-t^2s_2^2)}$$

Ignoring the multigrading by the two dimensional torus spanned by leaves (by setting $s_1=s_2=1$) we get:

$$h_{X(\text{⚲})}(t)=\frac{(1-t^2)\cdot(1-t^4)}{(1-t)^4\cdot(1-t^2)^3}=\frac{1+t^2}{(1-t)^4\cdot(1-t^2)}$$

We have seen in Example II.47 that $\tau(\text{-○-})$ has six generators: those are the elements in the above table for ⚲ apart from y_1. The model $X(\text{-○-})$ is a hypersurface of degree $(4,2,2)$ in $\mathbb{P}(1^4,2^2)$ so

$$h_{X(\text{-○-}),\mathcal{L}(\text{-○-})}(t,s_1,s_2)=\frac{(1-t^4s_1^2s_2^2)}{(1-t)^2\cdot(1-ts_1s_2)^2\cdot(1-t^2s_1^2)\cdot(1-t^2s_2^2)}$$
$$=h_{X(\text{⚲}),\mathcal{L}(\text{⚲})}(t,s_1,s_2).$$

Again we can ignore the multigrading and get

$$h_{X(\text{-○-})}(t)=\frac{(1-t^4)}{(1-t)^4\cdot(1-t^2)^2}=\frac{1+t^2}{(1-t)^4\cdot(1-t^2)}.$$

We expand to see the first few terms

$$h_{X(\text{⨀})}(t) = 1 + 4t + 12t^2 + 28t^3 + 57t^4 + 104t^5 + 176t^6 + 280t^7 + O(t^8).$$

Example IV.7. The Hilbert series of models of both graphs ⊖ and ⨀ with no leaves (thus no additional grading) and two cycles is

$$h_{X(\text{⨀})}(t) = h_{X(\ominus)}(t) = \frac{1}{(t^4 - 4t^3 + 6t^2 - 4t + 1)} = 1 + 4t + 10t^2 + 20t^3 + 35t^4 + 56t^5 + 84t^6 + 120t^7 + O(t^8).$$

This is because $X(\ominus)$ is $\mathbb{P}^3 = (\mathbb{P}^3 \times \mathbb{P}^3)/\!\!/(\mathbb{C}^* \times \mathbb{C}^* \times \mathbb{C}^*)$.

3. Computing the Hilbert function

Given a trivalent tree $\mathcal{T}$ with n leaves we computed the Hilbert function $H_{X(\mathcal{T})}$ of its model in [5] as

$$H_{X(\mathcal{T}),\mathbb{S}(\{l\})}(m,k) = 1_m^{\star n}(k),$$

where the additional grading corresponds to a distinguished leaf l, $\star$ is an appropriate summing formula and 1_m is the constant function. This inductive formula for $H_{X(\mathcal{T})}$ uses the decomposition of the tree $\mathcal{T}$ as a sum of tripods, which leads to the presentation of the polytope $\Delta(\mathcal{T})$ as a fiber product of tetrahedrons $\Delta(\text{⅄})$.

The same method works for any trivalent graph. We proved in Theorem IV.5 that the Hilbert function of mutation-equivalent graphs are equal. By Lemma II.11 we know that any graph is mutation-equivalent to a graph of the shape depicted on Figure IV.1.

Fig. IV.1.: Caterpillar graph

This means we have reduced the calculation to this case of caterpillar graphs. As we have described in Section 1, any graph is presented as union of tripods $\curlyvee$ with identifications. More precisely, any trivalent graph is built from $\curlyvee$ by the operations of grafting two graphs and gluing two leaves.

Remark IV.8. To produce a caterpillar graph $\mathcal{G}$ from |'s (leaves) and ♀'s (leaves with loop) using $\star$ and $\supset$, we need the second operation only once per graph and only in the case when $\mathcal{G}$ has no leaves.

Remark IV.9. On the level of graph models we have

$$X(\mathcal{G}_1 \star \mathcal{G}_2) = (X(\mathcal{G}_1) \times X(\curlyvee) \times X(\mathcal{G}_2)) /\!\!/ (\mathbb{C}^*)^2$$

and

$$X(\mathcal{G}^{l_1}_{l_2}\supset) = X(\mathcal{G}) /\!\!/ \mathbb{C}^*,$$

where the actions of the tori were described in Section II.3.3.

We give a formula for $h_{X(\mathcal{G}_1\star\mathcal{G}_2),\mathbb{S}(\mathcal{L}(\mathcal{G}_1\star\mathcal{G}_2))}$ and for $h_{X(\mathcal{G}^{l_1}_{l_2}\supset),\mathbb{S}(\mathcal{L}(\mathcal{G}^{l_1}_{l_2}\supset))}$, using the above fact about how the model of $\mathcal{G}_1 \star \mathcal{G}_2$ is constructed from smaller pieces.

$$h_{X(\mathcal{G}_1\star\mathcal{G}_2),\mathbb{S}(\mathcal{L}(\mathcal{G}_1\star\mathcal{G}_2))} = h_{X(\mathcal{G}_1),\mathbb{S}(\mathcal{L}(\mathcal{G}_1))} \star h_{X(\mathcal{G}_2),\mathbb{S}(\mathcal{L}(\mathcal{G}_2))} :=$$

$$\text{the part containing monomials of the form } (t_1t_2t_3)^i(s')^0(s'')^0(s''')^j s^I \text{of}$$

$$h_{X(\mathcal{G}_1)}(t_1, s_1, \ldots, s_{n_1}, \frac{1}{s'}) \cdot h_{X(\curlyvee)}(t_3, s', s'', s''') \cdot h_{X(\mathcal{G}_2)}(t_2, s_{n_1+1}, \ldots, s_{n_1+n_2}, \frac{1}{s''}) \tag{IV.10}$$

where $s = (s_1, \ldots, s_{n_2})$ and I is the exponent vector.

Let us compute the input functions: apart from the constant one which corresponds to leaves of $\mathcal{G}$ we have $H_{X(\varphi),\mathbb{S}(\{l\})}$ the Hilbert function of the model of graph with two edges. Recall that the model $X(\varphi)$ is $\mathbb{P}^3/\!\!/\mathbb{C}^* = \mathbb{P}(1,1,2)$, where the $\mathbb{C}^*$ action has weights $[010-1]$ on $\mathbb{P}^3$. Here is the list of generators with weights and the resulting graded Hilbert function

			
t	1	1	2
s	0	0	2

$\rightsquigarrow h(t,s) = \frac{1}{(1-t)(1-s^2t^2)}$

We can expand Formula (IV.10), setting f to be a Hilbert function of some graph, to get for $k \leq \frac{m}{2}$

$$\begin{aligned} h_{X(\varphi)} \star f(k) = (m-k+1) \sum_{a_0=0}^{m-k-1} f(a)[2|k+a](a+1)+ \\ (k+1) \sum_{a_0=m-k}^{k} f(a)[2|k+a](m+2-a)+ \\ k \sum_{a_0=k+1}^{m} f(a)[2|k+a](m+1-a) \end{aligned}$$

and for $k \geq \frac{m}{2}$

$$\begin{aligned} h_{\varphi} \star f(k) = (m-k+1) \sum_{a_0=0}^{m-k-1} f(a)[2|k+a](a+1)+ \\ (m-k+1) \sum_{a_0=m-k}^{k} f(a)[2|k+a](2m-2k-a+1)+ \\ (m-k) \sum_{a_0=k+1}^{m} f(a)[2|k+a](2m-2k-a) \end{aligned}$$

where $a = (a_0, a_1, \ldots, a_n)$.

In the same way we can write

$$h_{X(\mathcal{G}^{l_1}_{l_2\supset})}(t, s_1, \ldots, s_n) = \text{the part that contains monomials } t^i(s')^0 s^I \text{ of}$$
$$h_{X(\mathcal{G})}(t, s_1, \ldots, s_n, s', \frac{1}{s'}) \quad \text{(IV.11)}$$

where $s = (s_1, \ldots, s_n)$ and I is the exponent vector.

CHAPTER V

SUMMARY

We defined phylogenetic models on trivalent graphs by generalizing the quotient description of the binary symmetric models on trivalent trees. For the graphs with at most one cycle the set of minimal generators of the corresponding cone has a clear description. It remains an open question how to extend this result to all trivalent graphs.

We constructed torus invariant flat families inside some toric varieties which contain models of graphs with the same topological invariants. Moreover, we proved that they share the same multigraded Hilbert function. We provided an algorithm to compute it.

REFERENCES

[1] Elizabeth S. Allman and John A. Rhodes, *Phylogenetic ideals and varieties for the general Markov model*, Adv. in Appl. Math. **40** (2008), no. 2, 127–148. MR MR2388607 (2008m:60145)

[2] Andrzej Białynicki-Birula, *Quotients by actions of groups*, Algebraic quotients. Torus actions and cohomology. The adjoint representation and the adjoint action, Encyclopaedia Math. Sci., vol. 131, Springer, Berlin, 2002, pp. 1–82. MR MR1925829 (2003f:14055)

[3] Wieb Bosma, John Cannon, and Catherine Playoust, *The Magma algebra system. I. The user language*, J. Symbolic Comput. **24** (1997), no. 3-4, 235–265, Computational algebra and number theory (London, 1993). MR MR1484478

[4] Weronika Buczyńska, Maria Donten, and Jarosław A. Wiśniewski, *Isotropic models of evolution with symmetries*, Interactions of classical and numerical algebraic geometry, Contemp. Math., vol. 496, Amer. Math. Soc., Providence, RI, 2009, pp. 111–131. MR MR2555951

[5] Weronika Buczyńska and Jarosław A. Wiśniewski, *On geometry of binary symmetric models of phylogenetic trees*, J. Eur. Math. Soc. (JEMS) **9** (2007), no. 3, 609–635. MR MR2314109 (2008g:14090)

[6] Marta Casanellas, Luis David Garcia, and Seth Sullivant, *Catalog of small trees*, Algebraic statistics for computational biology, Cambridge Univ. Press, New York, 2005, pp. 291–304. MR MR2205880

[7] David Eisenbud, *Commutative algebra*, Graduate Texts in Mathematics, vol. 150,

Springer-Verlag, New York, 1995, With a view toward algebraic geometry. MR MR1322960 (97a:13001)

[8] Joseph Felsenstein, *Inferring phylogenies*, Sinauer Press, Sunderland, MA, 2004.

[9] William Fulton, *Introduction to toric varieties*, Annals of Mathematics Studies, vol. 131, Princeton University Press, Princeton, NJ, 1993, The William H. Roever Lectures in Geometry. MR MR1234037 (94g:14028)

[10] Alexander Grothendieck, *éléments de géometrie algébrique (rédigés avec la collaboration de jean dieudonné): Ii.étude globale élémentaire de quelques classes de mophismes*, Publications mathématique de l'IHÉS, Bures-sur-Yvette, France, 1961, Graduate Texts in Mathematics, No. 52.

[11] Mark Haiman and Bernd Sturmfels, *Multigraded Hilbert schemes*, J. Algebraic Geom. **13** (2004), no. 4, 725–769. MR MR2073194 (2005d:14006)

[12] Robin Hartshorne, *Connectedness of the Hilbert scheme*, Inst. Hautes Études Sci. Publ. Math. (1966), no. 29, 5–48. MR MR0213368 (35 #4232)

[13] ———, *Algebraic geometry*, Springer-Verlag, New York, 1977, Graduate Texts in Mathematics, No. 52. MR MR0463157 (57 #3116)

[14] Lisa C. Jeffrey and Jonathan Weitsman, *Bohr-Sommerfeld orbits in the moduli space of flat connections and the Verlinde dimension formula*, Comm. Math. Phys. **150** (1992), no. 3, 593–630. MR MR1204322 (94g:58085)

[15] Christopher A. Manon, *The algebra of conformal blocks*, arXiv:0910.0577v3 [math.AG], 2009.

[16] Ezra Miller and Bernd Sturmfels, *Combinatorial commutative algebra*, Graduate Texts in Mathematics, vol. 227, Springer-Verlag, New York, 2005. MR MR2110098 (2006d:13001)

[17] D. Mumford, J. Fogarty, and F. Kirwan, *Geometric invariant theory*, third ed., Ergebnisse der Mathematik und ihrer Grenzgebiete (2) [Results in Mathematics and Related Areas (2)], vol. 34, Springer-Verlag, Berlin, 1994. MR MR1304906 (95m:14012)

[18] Tadao Oda, *Convex bodies and algebraic geometry*, Ergebnisse der Mathematik und ihrer Grenzgebiete (3) [Results in Mathematics and Related Areas (3)], vol. 15, Springer-Verlag, Berlin, 1988, An introduction to the theory of toric varieties, Translated from the Japanese. MR MR922894 (88m:14038)

[19] Lior Pachter and Bernd Sturmfels, *Statistics*, Algebraic statistics for computational biology, Cambridge Univ. Press, New York, 2005, pp. 3–42. MR MR2205866

[20] Miles Reid, *Graded rings and birational geometry*, Proceedings of algebraic geometry symposium, Kinosaki, Oct 2000, K. Ohno (Editor), 2000, pp. 1–72.

[21] Charles Semple and Mike Steel, *Phylogenetics*, Oxford Lecture Series in Mathematics and its Applications, vol. 24, Oxford University Press, Oxford, 2003. MR MR2060009 (2005g:92024)

[22] Richard P. Stanley, *Hilbert functions of graded algebras*, Advances in Math. **28** (1978), no. 1, 57–83. MR MR0485835 (58 #5637)

[23] Bernd Sturmfels, *Gröbner bases and convex polytopes*, University Lecture Series, vol. 8, American Mathematical Society, Providence, RI, 1996. MR MR1363949

(97b:13034)

[24] Bernd Sturmfels and Seth Sullivant, *Toric ideals of phylogenetic invariants*, J. Comput. Biol. **12** (2005), no. 2, 204–228.

[25] Bernd Sturmfels and Zhiqiang Xu, *Sagbi basis and Cox-Nagata rings*, J. Eur. Math. Soc. (JEMS) **12** (2010), no. 2, 429–459.

VITA

Name:	Weronika Julia Buczyńska
Address:	Departement of Mathematics, Mechanics and Computer Science Warsaw University ul. Banacha 2 02-097 Warszawa, POLAND
Email Address:	wkrych@mimuw.edu.pl

Education: B.S in Computer Science, Warsaw University; 2001

M.S. in Mathematics, Warsaw University; 2002

Ph.D. in Mathematics, Texas A&M University, 2010