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Constructing algebraic varieties via finite group actions

PhD dissertation

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Author's declaration:
aware of legal responsibility I hereby declare that I have written this dissertation myself and all the contents of the dissertation have been obtained by legal means.

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Abstract

The aim of this thesis is to investigate certain properties of two constructions of algebraic varieties based on a finite group action.

In the first part we investigate Cox rings of minimal resolutions of (complex) surface quotient singularities $\mathbb{C}^2/G$, where G is a finite (small) subgroup of $GL(2,\mathbb{C})$. As a result we provide two descriptions of these rings. The first one is the single relation between its generators or, in other words, an equation for the spectrum of the Cox ring presented as a hypersurface in an affine space. In addition, we obtain an explicit description of the minimal resolution of $\mathbb{C}^2/G$ as a divisor in a toric variety. The second way of describing the Cox ring of the minimal resolution of $\mathbb{C}^2/G$ ring relies on viewing it as a subring of the coordinate ring of a product of a torus and another surface quotient singularity, $\mathbb{C}^2/[G,G]$. We give a method of finding a set of generators of such an embedding of the Cox ring, which uses only the information on the intersection numbers of components of the exceptional fibre of the considered resolution and on invariants of the induced action of $[G,G]$ on $\mathbb{C}^2$. We expect that this idea can be generalized to selected classes of resolutions of quotient singularities in higher dimensions.

The second part of the thesis concerns geometric models of Markov processes on phylogenetic trees. We concentrate on the case of phylogenetic trees with symmetries, understood as invariance with respect to a transitive action of a finite group. First we investigate the setting with added assumption of the isotropy of the model. The main result of this part concerns models with groups of symmetries containing large abelian subgroups. We prove that in this case the assumption of isotropy is unnecessary and we use these results to show that hyperbinary models are the only isotropic models with abelian group of symmetries.

Then we change the setting: we give up the assumption of isotropy and consider geometric properties of general group-based models and G-models. We give the first examples of non-normal models in these classes and compute Hilbert-Ehrhart polynomials to investigate the deformation equivalence of models for trees with the same number of leaves. Moreover, we propose a (conjectural) method of generating phylogenetic invariants of group-based models and prove that for the 3-Kimura model it is equivalent to an important conjecture of Sturmfels and Sullivant concerning the degree of generation of phylogenetic invariants.

Keywords: group action, invariant, symmetry, Cox ring, quotient singularity, resolution of singularities, toric variety, Markov process on a tree, phylogenetic tree, geometric model, model of evolution, general group-based model, phylogenetic invariant

AMS MSC 2010 classification: 14L30, 14E15, 14M25, 52B20, 13P25

Streszczenie

W niniejszej pracy doktorskiej badamy własności dwóch konstrukcji rozmaitości algebraicznych opartych na działaniu skończonej grupy.

Pierwsza część pracy dotyczy pierścieni Coxa minimalnych rozwiązań dwuwymiarowych osobliwości ilorazowych $\mathbb{C}^2/G$, gdzie G oznacza skończoną (małą) podgrupę $GL(2,\mathbb{C})$. Wynikiem są dwie metody opisu tych pierścieni. Pierwsza z nich to podanie (jedynej) relacji pomiędzy generatorami pierścienia Coxa lub, inaczej, równania opisującego zanurzenie spektrum tego pierścienia na hiperpowierzchnię w przestrzeni afinicznej. Dodatkowo otrzymujemy konstrukcję zanurzenia minimalnego rozwiązania $\mathbb{C}^2/G$ w trójwymiarową rozmaitość toryczną. Druga metoda badania struktury pierścieni Coxa minimalnego rozwiązania $\mathbb{C}^2/G$ opiera się na analizie włożenia tego pierścienia w pierścień współrzędnych produktu torusa i innej dwuwymiarowej osobliwości ilorazowej, $\mathbb{C}^2/[G,G]$. Podajemy metodę wyznaczania zbioru generatorów takiego zanurzenia pierścienia Coxa, która wymaga wyłącznie znajomości indeksów przecięć składowych dywizora wyjątkowego rozpatrywanego rozwiązania i struktury pierścienia niezmienników indukowanego działania $[G,G]$ na $\mathbb{C}^2$. Oczekujemy, że ten wynik uogólnia się na pewne klasy rozwiązań osobliwości ilorazowych w wyższych wymiarach.

W drugiej części pracy badamy modele geometryczne procesów Markowa na drzewach filogenetycznych. Zajmujemy się klasą drzew filogenetycznych z symetriami, rozumianymi jako niezmienniczość względem pewnego tranzytywnego działania skończonej grupy. Najpierw rozważamy przypadek z dodanym założeniem izotropowości modelu. Główny rezultat dotyczy klasy modeli z grupą symetrii zawierającą dużą podgrupę abelową. Dowodzimy, że w tym przypadku założenie izotropowości można pominąć, a ponadto wykorzystujemy otrzymane wyniki do wykazania, że modele hiperbinarne to jedyne izotropowe modele z abelową grupą symetrii.

Dalej rozpatrujemy inny przypadek: odrzucamy założenie izotropowości i badamy geometryczne własności drzew filogenetycznych z abelową grupą symetrii oraz z grupą symetrii zawierającą dużą normalną podgrupę abelową. Podajemy pierwsze przykłady takich drzew, których modele geometryczne nie są normalne. Obliczamy wielomiany Hilberta-Ehrharta pewnych modeli w celu badania ich deformacyjnej równoważności. Ponadto, podajemy (jako hipotezę) metodę znajdowania niezmienników filogenetycznych modeli z abelową grupą symetrii i dowodzimy, że dla modelu 3-Kimury jest ona równoważna znanej hipotezie Sturmfelsa i Sullivanta dotyczącej stopnia generatorów ideału niezmienników filogenetycznych.

Słowa kluczowe: działanie grupy, niezmiennik, symetria, pierścień Coxa, osobliwość ilorazowa, rozwiązanie osobliwości, rozmaitość toryczna, proces Markowa na drzewie, drzewo filogenetyczne, model geometryczny, model ewolucji, model z abelową grupą symetrii, niezmiennik filogenetyczny

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Contents

Chapter 1

Introduction

Group actions lead to many constructions of algebraic varieties. Symmetries coming from a group action appearing in such a construction are a powerful tool for understanding the structure of geometric objects. Therefore, whenever a group action is involved in a definition of a class of varieties, one may hope that it will be an interesting topic of studies. In particular, investigating objects endowed with a group action often lead to finding new examples of classes defined by some specific properties. Also, the presence of symmetries usually reduces complexity of considered objects. From numerous possibilities of realizing these ideas let us mention here only these which have a direct impact on the content of the present thesis.

A natural problem is to consider quotients of varieties by group actions (although defining the quotient by a group action in algebraic geometry is in general a nontrivial problem). The simplest examples are quotients of affine spaces by finite group actions. Properties of such quotients in dimension two, i.e. surface quotient singularities, are investigated in the first part of the thesis. More precisely, the objects we study are the Cox rings of minimal resolutions of these singularities. A very important observation is that considered resolutions can be constructed as quotients of affine varieties corresponding to their Cox rings by a torus action.

This topic should be viewed in the context of the Kummer construction of a K3 surface, see [Kum75], and its generalizations, useful for instance to construct Calabi-Yau varieties important from the point of view of the string theory. From such a generalization of the Kummer construction, introduced in [AW10] and investigated also in [Don11], originated the first part of this work.

In the second part of the thesis we consider geometric models of Markov processes on phylogenetic trees, that is algebraic varieties associated with certain combinatorial structures containing the data of an evolution process. From the general class of such structures we chose these which are endowed with a finite group action of a certain type and attempt to understand algebraic and geometric properties of corresponding varieties. Results of the research in this area (see e.g. [SS05, DK09, Mic11a]), including our results presented in chapters 7 and 8, show clearly that quite often it is possible to obtain some information on models with a group action, while very little can be said on the phylogenetic models in their full generality.

Another class of varieties constructed using a group action, non-finite this time, are toric varieties. The torus action with an open orbit allows to give a useful combinatorial description of such varieties. Moreover, any normal toric variety can be constructed as a quotient of an open subset of an affine space by a torus action (as described in section 2.2), which is an important point in the first part of the thesis. Although toric varieties are not constructed via a finite group action, we mention them here, since they make a very significant tool in both parts of our work. Their properties used throughout the thesis are collected in chapter 2.
It may seem that the two topics considered in the thesis, the Cox rings of minimal resolutions of surface quotient singularities and geometric models of phylogenetic trees with symmetries, have little in common apart from using the group action in definitions of investigated objects. However, it turned out that they both can be approached using methods of toric geometry, which has made it much easier to work on these problems concurrently. Moreover, in fact a direct link between these two topics exists: as explained in [SX10], binary (i.e. with an action of $\mathbb{Z}_2$) phylogenetic models are connected to degenerations of the spectra of Cox rings on blow-ups of projective spaces.
Next two sections are separate introductions to both parts of the thesis and in section 1.3 we collect basic definitions concerning group actions.

Throughout the thesis we work over the field of complex numbers $\mathbb{C}$, that is we consider only complex algebraic varieties.

1.1 Cox rings of minimal resolutions of surface quotient singularities

The Cox ring (or the total coordinate ring) of a normal algebraic variety can be defined as the $\mathrm{Cl}(X)$-graded module

$$\mathrm{Cox}(X) = \bigoplus_{[D]\in \mathrm{Cl}(X)} \Gamma(X, \mathcal{O}_X(D)),$$

with multiplication as in the ring of rational functions on X; for the details of the definition see section 3.5. One can look at $\mathrm{Cox}(X)$ from a geometric point of view if only it is finitely generated. Assume $\mathrm{Pic}(X)$ is torsion-free and consider the action of the Picard torus of X

$$T = \mathrm{Hom}(\mathrm{Pic}(X), \mathbb{C}^*)$$

on $\mathrm{Spec}(\mathrm{Cox}(X))$. Then X can be obtained as a geometric quotient of an open subset of $\mathrm{Spec}(\mathrm{Cox}(X))$ by T. Thus the Cox ring contains a lot of information on the geometry of X – the variety is determined by $\mathrm{Cox}(X)$ and some combinatorial data in its grading group (see e.g. [LV09]).
In chapters 3-5 we study minimal resolutions of complex surface quotient singularities: X denotes the minimal resolution of the quotient $\mathbb{C}^2/G$ for a finite (small) subgroup $G \subset GL(2, \mathbb{C})$. The aim of our work is to understand Cox rings of these

resolutions: to show that they are finitely generated and to describe them in terms of generators and relations. Note that in our case the Picard torus action can be considered because for the minimal resolution X of $\mathbb{C}^2/G$ the class group $\mathrm{Cl}(X) = \mathrm{Pic}(X)$ is torsion-free by Proposition 3.4.9.

Motivation, state of the art

This work can be thought of as a first step towards understanding the total coordinate rings of resolutions of quotient singularities also in higher dimensions. An important motivation for this problem is the possibility of presenting X as a geometric quotient of an open set of $\mathrm{Spec}(\mathrm{Cox}(X))$ in case where $\mathrm{Cox}(X)$ is finitely generated. Roughly speaking, if one finds a way to understand the Cox ring of a (hypothetical) resolution X of a (quotient) singularity, based only on some restricted knowledge of the geometry of X, one may be able to construct some new resolutions as geometric quotients of open sets of $\mathrm{Spec}(\mathrm{Cox}(X))$. Recall that in higher dimensions the notion of the minimal resolution of the singularity, although it may be defined in the context of the minimal model theory (so that the canonical divisor is relatively nef), it does not yield a unique resolution. In fact, there may be a number of resolutions, or partial resolutions, which are isomorphic in codimension 1 and are related by so-called flops, see e.g. [Rei92]. Nevertheless, such resolutions should share the same Cox ring, which makes studying this object even more sensible. An especially interesting case is the one of 4-dimensional symplectic quotient singularities and their symplectic resolutions. The continuation of the project started in this thesis is a joint work in progress with J. Wiśniewski, [DBW13].
Another motivation for investigating Cox rings of resolutions of quotient singularities comes from more complex quotient constructions of algebraic varieties, in particular a generalization of the Kummer construction proposed in [AW10]. The initial idea of extending the results of [Don11] by finding the Cox rings of Kummer 3-folds (constructed by resolving singularities of certain quotients of an abelian variety by finite group actions) evolved to the question about the local situation, which turned out to be at least as interesting as the original one. Therefore in this thesis we consider only affine quotients by a group action, but applying these results to finding Cox rings of generalized Kummer varieties seems an interesting problem for the future work.
At the moment not much is known about Cox rings of resolutions of quotient singularities. The first attempt to study these objects is a recent paper [FGAL11], where the authors find the single relation of $\mathrm{Cox}(X)$ where X is the minimal resolution of a Du Val singularity (i.e. $G \subset SL(2, \mathbb{C})$). However, their methods rely heavily on the equations of an embedding of the singularity in an affine space, and consequently their work seems to be very hard to generalize. Cox rings of minimal resolutions of all surface quotient singularities can also be described using the theory of varieties endowed with a (diagonal) torus action such that its biggest orbits are of codimension one, see [HS10]. However, these results also do not apply to singularities in higher dimensions, hence they are not really useful for us, since our primary goal is to develop a method which will work also in a more general setting.

Results and organization of work

In chapter 3 we present the details of our setting. We recall the classification of surface quotient singularities and describe their minimal resolutions (after [Bri68]). Then basic information on the Cox rings (after [ADHL10]), which will be used in the following chapters, is collected in section 3.5.

In chapter 4 we prove the first of the main results of this part, Theorem 4.3.3. This requires a lot of preparatory work. In section 4.1 we define an action of the Picard torus T of the minimal resolution X on an affine space which then becomes the ambient space for $\mathrm{Spec}(\mathrm{Cox}(X))$. We analyze properties of this action in the toric setting and describe the quotient as a toric variety. Then a candidate S for $\mathrm{Spec}(\mathrm{Cox}(X))$ is proposed; it is defined as a T-invariant hypersurface in an affine space.

Section 4.2 is devoted to describing a geometric quotient of an open subset of S by the action of T as a divisor in a toric variety. We prove that it is the minimal resolution of $\mathbb{C}^2/G$, which is the main step in the proof of Theorem 4.3.3. This may seem to be a roundabout way of reproving the results of [Bri68]. However, this point of view on the problem is justified, since we are planning to use the ideas developed in this work in cases of higher dimensional quotient singularities, where resolutions do not have such a detailed description, and try to reverse the process: construct resolutions of quotient singularities from their Cox rings.

The main result of chapter 4, Theorem 4.3.3, states that S is the spectrum of the Cox ring of X. Hence $\mathrm{Spec}(\mathrm{Cox}(X))$ is a hypersurface in an affine space, given by a single equation which can be easily written down using the description of the exceptional divisor of the minimal resolution of $\mathbb{C}^2/G$ (for the details see Construction 4.1.22). The proof is based on [ADHL10, Thm. 6.4.3], the GIT characterization of the Cox ring.

Chapter 5 discusses an even more important result, Theorem 5.2.9. It is a description of $\mathrm{Cox}(X)$ in terms of its generators, as a subring of $\mathbb{C}[x,y]^{[G,G]} \otimes \mathbb{C}[t_0^{\pm 1}, \ldots, t_{n-1}^{\pm 1}]$, where $[G,G]$ denotes the commutator subgroup of G. After presenting the proof, in section 5.3, we give a few examples of sets of generators of the Cox rings in some specific cases.

While Theorem 4.3.3 is related to the results of [HS10] and can be proven using the ideas similar to the ones presented there, Theorem 5.2.9 introduces a new method of describing the Cox ring, designed to work also in the case of quotient singularities in higher dimensions. The ideas described in chapter 5 are generalized and applied to higher-dimensional singularities in [DBW13]. As in the present thesis we develop methods which should work also in a more general situation, we do everything step by step, performing quite a lot of computations, checking details and providing examples.

1.2 Models of evolution with symmetries

In chapters 6-8 we consider a few problems inspired by questions from algebraic statistics. The objects we investigate are geometric models of Markov processes on phylogenetic trees. The nature of such a structure depends on three elements. Firstly, we fix a finite set $\mathcal{A}$. Its elements, called letters, correspond to features whose evolution we are modeling. For example, they can be the four letters A, C, T, G, which usually stand for the nucleotides in the DNA. The second element is a tree (i.e. an acyclic graph) $\mathcal{T}$. To its vertices we assign random variables, which take values in $\mathcal{A}$, describing the states of the process. Finally, we choose a model of evolution (usually written in the form of a space of matrices), which defines the rules of possible modification of random variables assigned to the vertices while passing from one vertex to another along an edge of $\mathcal{T}$. In other words, the model of evolution can be understood as a space parameterizing possible values of the conditional probability relating variables associated with ends of an edge of $\mathcal{T}$.
With such a process one can associate a geometric model – an algebraic variety which contains information about a possible distribution of the letters over the leaves of the tree $\mathcal{T}$. The details of this construction are given in section 6.2. In the thesis we concentrate on investigating phylogenetic trees from the point of view of algebraic geometry, i.e. we try to understand properties of their geometric models. While the biological and statistical connotations have significant influence on the definition of the structure we consider, they are not necessary for describing the mathematical results. Hence we give only a few words of explanation of the context in section 6.3, and for a more comprehensive discussion we advise the reader to look into one of the standard references in the field, for example [SS03] or [PS05, Part I].
In natural sciences symmetries are often used to reduce complexity of a problem. It turns out that it works very well in the case of phylogenetic trees – restricting to the class of models of evolution with symmetries (given by a finite group action), or to its subclasses, lead to a lot of interesting results, which do not apply to more general trees. Moreover, there are models, closely related to biological origins of this field, which have symmetries implied in a natural way by biochemical constraints. Therefore we concentrate on investigating properties of geometric models of phylogenetic trees with symmetries.

Symmetric models: state of the art

The class of models of evolution with symmetries which appears most frequently in the literature is the class of general group-based models. The group of symmetries, which acts transitively and effectively on the set $\mathcal{A}$ of letters, is there assumed to be an abelian group. It was introduced in [ES93] and [SSE93], and investigated later by other authors. For instance, in [SS05] algebraic and geometric properties of these models are considered. In particular, it was observed that algebraic varieties associated with general group-based models are toric varieties, which opens a possibility of applying methods of toric geometry to phylogenetic trees.
In chapter 8 we concentrate mainly on general group-based models. However, some

of the results presented there concerns a bigger class of so-called G-models. These are models which, apart from a transitive and effective action of an abelian group on $\mathcal{A}$, have some additional symmetries consistent with the abelian group action; for the precise definition see section 6.4. They were introduced by M. Michałek, the coauthor of the results of chapter 8, in his doctoral thesis [Mic12b] and the paper [Mic11a]. However, his definition is based on the ideas presented in chapter 7 on this thesis, coming from a joint work with W. Buczyńska and J. Wiśniewski, [BDW09].
The work presented in chapter 7 uses more general assumptions on the group of symmetries of a model (we require only the transitiveness and effectiveness of the action on $\mathcal{A}$), but we add an assumption of the isotropy of a model. By this we mean that the edges of the tree $\mathcal{T}$ are not directed (hence $\mathcal{T}$ can be unrooted) and the matrices describing conditional probability are symmetric. This assumption corresponds to the time-reversibility of the Markov process. The aim of this work was to develop a good setting, and to find a sensible class of models, for further investigation by means of algebraic geometry (and, in fact, it gave the first idea for distinguishing the class of G-models). Hence the character of the results described in chapter 7 is more algebraic and combinatorial.
In section 6.4.2 we briefly describe other classes of symmetric models of evolutions which can be found in the literature, but only these mentioned above are investigated in this thesis.

Results and organization of work

Chapter 6 is the introduction to the second part of the thesis. We describe there the details of the construction of phylogenetic trees and of their geometric models. Then we add a few words on the biological motivation for considering these structures and finish with discussing phylogenetic trees with symmetries.
At the beginning of chapter 7, devoted to investigating isotropic models of evolution, we collect basic observations which follow from the construction of such models and will be referred to. In section 7.2 we consider hyperbinary models of evolution, which have the group of symmetries equal to $\mathbb{Z}_2^s$ and generalize the binary model investigated in [BW07]. This section ends with Theorem 7.2.10, which explains the importance of hyperbinary models – the result is that these are the only isotropic models with abelian groups of symmetries. The proof of this theorem is based on observations made in section 7.3, where we investigate isotropic models of evolution whose group of symmetries G has an abelian subgroup H acting transitively and effectively on the set $\mathcal{A}$ of letters. Proposition 7.3.6, which states that for this kind of models the assumption of isotropy is unnecessary, gave the idea for investigating the class of G-models. The last section of this chapter contains a large set of examples of isotropic models with symmetries, prepared in the form of classification of such models for the set $\mathcal{A}$ small enough.
Chapter 8 concerns mainly geometric properties of varieties associated with general group-based models and G-models. To be able to predict some results or to construct counterexamples we made computational experiments. Our software, based

on the algorithm proposed in [Mic11a], which produces a toric description of a geometric model of a phylogenetic tree with symmetries (i.e. the corresponding lattice polytope) is described in section 8.1. In the next two sections we discuss some applications of computational tools to the questions about normality and deformation equivalence of general group-based models and selected G-models. Our results are summarized in Proposition 8.2.2 and Proposition 8.3.3. The topic of section 8.4 is one of the most important questions in this area: determining generators of the ideal of phylogenetic invariants of a model (i.e. the ideal of polynomials vanishing on the geometric model). Inspired by conjectures stated in an influential paper [SS05], we propose a (conjectural) method of obtaining phylogenetic invariants of claw trees (trees with only one inner vertex), which is the only missing step in understanding phylogenetic invariants of any tree, see Conjecture 8.4.9. What is important, this method is not purely algebraic, but involves looking at the geometry of considered varieties. In Proposition 8.4.17 we prove that Conjecture 8.4.9 holds in the simplest case – for the binary model. Moreover, in Propositions 8.4.13 and 8.4.19 we relate this conjecture to the ones of [SS05].

1.3 Group actions: notation and basic facts

The following notation will be used throughout the thesis.

- The unit of a group is most often denoted by 1 when we use the multiplicative notation and by 0 when the notation is additive. Sometimes, when we think of a matrix group or a transformation group, we denote it by id.
- By writing $H \subset G$ or $H \subseteq G$, where G is a group, we mean a group inclusion, that is H is a subgroup of G (unless explicitly stated otherwise – in section 7.3 we consider two groups, one embedded in the other just as sets, not by a group homomorphism).
- Let G act on a set X; the action on $x \in X$ is denoted by $g(x)$ or $g \cdot x$. The **orbit** of x, denoted by $G \cdot x$, is the set $\{g(x) \colon g \in G\} subset X$. The **isotropy group** of x, denoted by G_x, is the subgroup $\{g \in G \colon g(x) = x\} \subset G$.
- We say that $g \in G$ fixes $x \in X$ if $g(x) = x$. Then x is a **fixed point** of the action of G if all $g \in G$ fix x.
- The action of G on X is called **transitive** if it has exactly one orbit.
- The action of G on X is called **effective** if the only $g \in G$ which fixes all $x \in X$ is $g = 1$.
- The action of G on X is called **free** if the only $g \in G$ which fixes some $x \in X$ is $g = 1$.
- A **linear representation** of G is a vector space V with a homomorphism $\rho \colon G \to GL(V)$ defining the linear action of G on V.

In what follows we will refer to the statements given below.

Lemma 1.3.1. *Let G be an abelian group which acts effectively and transitively on a finite set X. Then this action is equivalent to the action of G on itself. More precisely, choosing an element in X and identifying it with the unit of G gives a bijection $G \longrightarrow X$ such that the action $G \times X \longrightarrow X$ is identified with multiplication $G \times G \longrightarrow G$.*

Proof. Since G is abelian, it acts on the set of fixed points of any $g \in G$, hence by the transitivity of the action this set is either empty or X. ☐

Definition 1.3.2. The **regular representation** of G is constructed as follows: the space V is spanned by a set $\{e_g \colon g \in G\}$ and the action of G on V is given by

$$h(\sum_{g \in G} c_g e_g) = \sum_{g \in G} c_g e_{hg}.$$

Lemma 1.3.3. *The regular representation $\rho_G : G \longrightarrow GL(V)$ can be diagonalized in terms of characters of G. That is, ρ_G is equivalent to $\rho_G^\chi : G \longrightarrow GL(V)$ such that for every $g \in G$ it holds $\rho_G^\chi(g) = \mathrm{diag}(\chi_i(g))$, where* diag *stands for a diagonal matrix and χ_i runs over all different characters in the dual group $G^\vee = \mathrm{Hom}(G, \mathbb{C}^*)$.*

For the proof see e.g. [FH91, Cor. 2.18].

Chapter 2

Toric varieties

Toric geometry is one of the most important tools in both parts of this thesis. The aim of this chapter is to recall briefly its language and present a few necessary definitions and theorems on toric varieties, based on [CLS11] and [Ful93]. First, for the convenience of the reader, we collect most frequently used definitions and notation in one place. After an introductory section we describe the quotient construction of a toric variety (see eg. [CLS11, Sect. 5.1]) and its corollaries. These results will be used mainly in Chapter 4 to construct certain embeddings of resolutions of quotient singularities in toric varieties, associated with the structure of their Cox rings. Then, in Section 2.3, we collect definitions and facts concerning toric varieties associated with lattice polytopes and normality of toric varieties, which will be used in chapter 8.

2.1 Basic facts

Throughout the thesis by a variety we understand a separated algebraic variety. We will consider only varieties over $\mathbb{C}$.

Definition 2.1.1. [CLS11, Def. 3.1.1] A toric variety is an irreducible variety X containing a torus $T_N \simeq (\mathbb{C}^*)^n$ as a Zariski open subset such that the action of T_N on itself extends to an algebraic action of T_N on X, i.e. the action $T_N \times T_N \to T_N$ extends to a morphism $T_N \times X \to X$.

In the first part of the thesis (chapters 3-5) all considered toric varieties will be normal. Such varieties can be can be described combinatorially by giving a fan of convex polyhedral cones (see e.g. [CLS11, Cor. 3.1.8]). Hence the notation for this construction, given below, will be used much more frequently than the definition above.

Notation 2.1.2. We use the following notation for toric varieties:

- By N we denote the **lattice of one-parameter subgroups** of an algebraic torus, and by M the dual lattice $\mathrm{Hom}(N, \mathbb{Z})$, i.e. the **monomial lattice** of the torus. The torus associated with these lattices can be written as

$$T_N = N \otimes_{\mathbb{Z}} \mathbb{C}^* = \mathrm{Hom}_{\mathbb{Z}}(M, \mathbb{C}^*).$$

- By a **cone** we mean a strongly convex rational polyhedral cone in a vector space $N_{\mathbb{R}} = N \otimes \mathbb{R}$, i.e. a subset $\sigma \in N_{\mathbb{R}}$ such that there are vectors $v_1, \ldots, v_n \in N$ such that any point $x \in \sigma$ can be presented as $x = \sum a_i v_i$ for some $a_1, \ldots, a_n \in \mathbb{R}_{\geq 0}$. A cone spanned by vectors $v_1, \ldots, v_n$ is denoted by $\sigma(v_1, \ldots, v_n)$ or $\mathrm{Cone}(v_1, \ldots, v_n)$.

- We say that a cone σ has **dimension** n if its points span an n-dimensional vector space. Hence σ is of maximal dimension if it spans $N_{\mathbb{R}}$.

- A **ray** is a one-dimensional cone, most often denoted by ρ. A **ray generator** u_ρ is the generator of the semigroup $\rho \cap N$.

- A **dual cone** to $\sigma \subset N_{\mathbb{R}}$ is $\sigma^\vee = \{m \in M_{\mathbb{R}} \colon \langle m, u \rangle \geq 0 \ \forall u \in \sigma\}$.

- A cone τ is a **face** of σ (denoted $\tau \preccurlyeq \sigma$) if it can be presented as $\sigma \cap H_m$, where H_m is a hyperplane in $N_{\mathbb{R}}$ orthogonal to some $m \in \sigma^\vee$. If σ is n-dimensional, then its **facets** are faces of dimension $n-1$.

- Take a cone $\sigma \subset N_{\mathbb{R}}$; an **affine toric variety** U_σ is an affine variety whose coordinate ring is a subring of the coordinate ring of the torus generated by monomials corresponding to the points of $\sigma^\vee \cap M$. If τ is a face of σ is a face then there is a natural embedding $U_\tau \subset U_\sigma$ to an open subset. In particular, $T_N \subset U_\sigma$ since it corresponds to the zero cone. By construction of U_σ the action of T_N on itself extends uniquely to the action on U_σ, compatible with the embeddings $U_\tau \subset U_\sigma$ corresponding to faces of σ.

- A **fan** Σ in $N_{\mathbb{R}}$ is a finite collection of cones such that for any $\sigma \in \Sigma$ all its faces are also in Σ and the intersection $\sigma \cap \tau$ of any two $\sigma, \tau \in \Sigma$ is a face of each. By $\Sigma(n)$ we denote the set of n-dimensional faces of Σ.

- A **toric variety of a fan** $\Sigma \subset N_{\mathbb{R}}$, denoted X_Σ, is constructed by gluing all U_σ for $\sigma \in \Sigma$ along open subsets corresponding to common faces. Since the gluing is compatible with the T_N-action, X_Σ is also endowed with the action of T_N. By [CLS11, Thm. 3.1.5] through this construction we obtain separated normal varieties. Any separated normal toric variety can be obtained this way.

- We say that X_Σ has **no torus factors** if $N_{\mathbb{R}}$ is spanned by the sets of ray generators of Σ.

A morphism of toric varieties $\phi \colon X_{\Sigma_1} \to X_{\Sigma_2}$, where Σ_i is a fan in $(N_i)_{\mathbb{R}}$, is toric (i.e. is a morphism in the category of toric varieties) if it maps T_{N_1} to T_{N_2} and $\phi|_{T_{N_1}} : T_{N_1} \to T_{N_2}$ is a group homomorphism. In case of normal toric varieties this condition translates to the combinatorial language as follows.

Theorem 2.1.3. *[CLS11, Thm. 3.3.4] Using the notation above, ϕ is a toric morphism if and only if the induced $\mathbb{Z}$-linear map*

$$\overline{\phi} \colon N_1 \to N_2$$

is compatible with the fans Σ_1, Σ_2, *i.e. for every cone* $\sigma_1 \in \Sigma_1$ *there exists a cone* $\sigma_2 \in \Sigma_2$ *such that* $\overline{\phi}_{\mathbb{R}}(\sigma_1) \subseteq \sigma_2$.

We will use a few another observations connecting the geometry of a toric variety to the combinatorics of its fan.

Definition 2.1.4. A cone is **smooth (or regular)** if its ray generators form a part of a $\mathbb{Z}$-basis of N. It is **simplicial**, if its ray generators are linearly independent over $\mathbb{R}$.
We say that a fan Σ is smooth (simplicial) if every cone of Σ is smooth (simplicial). And we say that Σ is complete if its cones sum up set-theoretically to the whole $N_{\mathbb{R}}$.

Theorem 2.1.5. *[CLS11, Thm 3.1.19] Let* Σ *be a fan in* $N_{\mathbb{R}}$ *and* X_Σ *the corresponding toric variety. Then*

1. X_Σ *is smooth if and only if* Σ *is smooth,*
2. X_Σ *has only finite quotient singularities if and only if* Σ *is simplicial,*
3. X_Σ *is compact in the classical topology if and only if* Σ *is complete.*

Example 2.1.6. [CLS11, Ex. 3.1.16] As an example we describe Hirzebruch surface F_r using the toric language. By $\{e_1, e_2\}$ we denote the standard basis of $N \simeq \mathbb{Z}^2$. Let $\Sigma_r \subset \mathbb{R}^2$ be the fan consisting of $\mathrm{Cone}(e_1, e_2)$, $\mathrm{Cone}(e_1, -e_2)$, $\mathrm{Cone}(re_2 - e_1, e_2)$, $\mathrm{Cone}(re_2 - e_1, -e_2)$ and all their faces, as in Fig. 2.1.

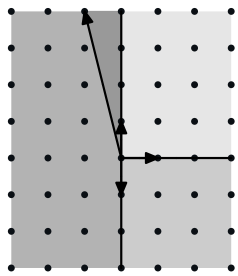


Figure 2.1: The fan of a Hirzebruch surface F_4

It is a smooth complete toric surface. The projection of N along e_2 onto $span(e_1)$ gives a morphism of Σ_r onto the fan of $\mathbb{P}^1$ (consisting of $\mathrm{Cone}(e_1)$, $\mathrm{Cone}(-e_1)$ and the zero cone in $\mathbb{Z}$). This is a $\mathbb{P}^1$-bundle and the orbits in $X(\Sigma_r)$ corresponding rays $\rho(e_1)$ and $\rho(re_2 - e_1)$ are its torus invariant fibers.

Finally, we recall the description of Weil divisors, the class group and Cartier divisors of a toric variety X_Σ. It will be important later that the class group of a toric variety is generated by classes of T_N-invariant Weyl divisors.

Definition 2.1.7. The class group $\mathrm{Cl}(X)$ of a normal algebraic variety X is the quotient $\mathrm{Div}(X)/\mathrm{Div}_0(X)$ of the group of all Weil divisors on X by the principal divisors subgroup.

Let D_ρ be the torus invariant prime divisor coming from the ray $\rho \in \Sigma(1)$ by the orbit-cone correspondence (see eg. [CLS11, Thm. 3.2.6]). Then the subgroup of $\mathrm{Div}(X_\Sigma)$ of all torus invariant divisors is

$$\mathrm{Div}_{T_N}(X_\Sigma) = \bigoplus_{\rho \in \Sigma(1)} \mathbb{Z} D_\rho.$$

Theorem 2.1.8. *[CLS11, Thm 4.1.3] If X_Σ is a toric variety without torus factors. Then there is a short exact sequence*

$$0 \longrightarrow M \longrightarrow \mathrm{Div}_{T_N}(X_\Sigma) \longrightarrow \mathrm{Cl}(X_\Sigma) \longrightarrow 0.$$

(If X_Σ has torus factors, it is not exact on the left.)

Proposition 2.1.9. *[CLS11, Thm 4.2.8] Let $D = \sum_{\rho \in \Sigma(1)} a_\rho D_\rho$ be a torus invariant Weil divisor. Then it is Cartier if and only if it can be there is a set of characters $\{m_\sigma : \sigma \in \Sigma_{max}\} \subset M$ such that*

$$\langle m_\sigma, u_\rho \rangle = -a_\rho$$

for all $\rho \in \sigma(1)$, where u_ρ is the primitive generator of the ray ρ.

Proposition 2.1.10. *[CLS11, Prop. 4.2.7] The fan Σ is simplicial if and only if X_Σ is $\mathbb{Q}$-factorial, i.e. every Weil divisor on X_Σ has a positive integer multiple that is Cartier.*

Remark 2.1.11. If X_Σ is $\mathbb{Q}$-factorial then every Weil divisor has a description as in Proposition 2.1.9, but m_σ have rational coefficients, that is $\{m_\sigma : \sigma \in \Sigma_{max}\} \subset \mathbb{Q} \cdot M$.

2.2 The quotient construction

There is a canonical way of presenting a toric variety as a quotient of an open subset of an affine space. We use it to construct an ambient space for a quotient of the spectrum of a Cox ring in Chapter4. The result is recalled below and all the details can be found in [CLS11, Sect. 5.1].
Before returning to the toric setting we explain what kind of quotients are considered.

Definition 2.2.1. Let G be a group acting on an algebraic variety X. Then a morphisms $\pi : X \to Y$ is a **good categorical quotient**, if

1. it is constant on orbits of G,
2. if $U \subseteq Y$ is open, then the natural map $\mathcal{O}_Y(U) \longrightarrow \mathcal{O}_X(\pi^{-1}(U))$ induces an isomorphism $\mathcal{O}_Y(U) \simeq \mathcal{O}_X(\pi^{-1}(U))^G$,
3. for each $W \subseteq X$ closed and G-invariant $\pi(W) \subseteq Y$ is closed,
4. if W_1 and W_2 are closed, disjoint and G-invariant in X, then $\pi(W_1)$ and $\pi(W_2)$ are disjoint in Y.

In this situation we denote the quotient space Y by $X /\!/ G$.

Definition 2.2.2. Let $\pi\colon X \to X/\!/G$ be a good categorical quotient. It is called a **geometric quotient**, denoted by X/G, if fibers of π are single G-orbits (or, equivalently, if all G-orbits in X are closed).
We say that π is an **almost geometric quotient** if $X/\!/G$ has a Zariski dense open subset U such that $\pi|_{\pi^{-1}(U)}\colon \pi^{-1}(U) \to U$ is a geometric quotient.

Let X_Σ be the toric variety of a fan Σ in $N_\mathbb{R}$. We assume that X_Σ has no torus factors, which is sufficient for our applications. However, in [CLS11, Sect. 5.1] the case of varieties with torus factors is also discussed.
The group whose quotient we consider in the construction is

$$G = \mathrm{Hom}_\mathbb{Z}(\mathrm{Cl}(X_\Sigma), \mathbb{C}^*).$$

It appears naturally in the exact sequence constructed by applying $\mathrm{Hom}_\mathbb{Z}(-, \mathbb{C}^*)$ to the exact sequence in Theorem 2.1.8

$$1 \longrightarrow G \longrightarrow (\mathbb{C}^*)^{|\Sigma(1)|} \longrightarrow T_N \longrightarrow 1.$$

Take the polynomial ring

$$S = \mathbb{C}[x_\rho\colon \rho \in \Sigma(1)].$$

For each $\sigma \in \Sigma$ we define the monomial

$$x^{\widehat{\sigma}} = \prod_{\rho \notin \sigma} x_\rho \in S.$$

Definition 2.2.3. The ideal $B(\Sigma) = \langle x^{\widehat{\sigma}}\colon \sigma \in \Sigma \rangle \subseteq S$ is called the **irrelevant ideal**. Its zero set in $\mathrm{Spec}(S) = \mathbb{C}^{|\Sigma(1)|}$ is denoted by $Z(\Sigma)$.

Let $e_\rho\colon \rho \in \Sigma(1)$ be the standard basis of the lattice $\mathbb{Z}^{|\Sigma(1)|}$. We start from defining a toric morphism

$$\pi\colon \mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma) \to X_\Sigma.$$

We lift every $\sigma \in \Sigma$ to $\mathbb{R}^{|\Sigma(1)|}$ taking $\widetilde{\sigma} = \mathrm{Cone}(\{e_\rho\colon \rho \in \sigma(1)\})$. All such liftings form a fan $\widetilde{\Sigma}$ in $\mathbb{R}^{|\Sigma(1)|}$ which, by [CLS11, Prop. 5.1.9], gives the toric variety $\mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma)$. Moreover, the fan homomorphism from $\widetilde{\Sigma}$ to Σ sending $e_\rho \in \mathbb{Z}^{|\Sigma(1)|}$ to $u_\rho \in N$ induces the desired toric morphism π.

Theorem 2.2.4. *[CLS11, Thm. 5.1.11] Let X_Σ be a toric variety without torus factors. Consider the toric morphism $\pi\colon \mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma) \to X_\Sigma$ defined above. Then*

1. *π is an almost geometric quotient for the action of G on $\mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma)$. Thus*

$$X_\Sigma \simeq (\mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma)) /\!/ G.$$

2. *π is a geometric quotient if and only if Σ is simplicial.*

Remark 2.2.5. The ring $S = \mathbb{C}[x_\rho \colon \rho \in \Sigma(1)]$ is the total coordinate ring for X_Σ, as it will be defined in section 3.5. The quotient construction presented above is the simplest case of a general idea of presenting a variety as a quotient of the spectrum of its Cox ring by torus action. More details on such a quotient presentation are provided in Section 3.5. In section 3.3, where we briefly discuss the case of cyclic quotient singularities, we return to the total coordinate ring of a toric variety.

The quotient construction has a nice consequence, which simplifies working in local coordinates on a toric variety. As before, let X_Σ be a toric variety without torus factors. For a cone $\sigma \in \Sigma$ consider a map $\phi_\sigma \colon \mathbb{C}^{|\sigma(1)|} \to \mathbb{C}^{|\Sigma(1)|}$, which takes a point $(a_\rho)_{\rho\in\sigma(1)}$ to $(b_\rho)_{\rho\in\Sigma(1)}$ such that

$$b_\rho = \begin{cases} a_\rho & \rho \in \sigma(1); \\ 1 & \text{otherwise.} \end{cases}$$

Proposition 2.2.6. *[CLS11, Prop. 5.2.10] In the setting as above let $\sigma \in \Sigma$ be a smooth cone of maximal dimension. Then there is a commutative diagram*

$$\begin{array}{ccc} \mathbb{C}^{|\sigma(1)|} & \xrightarrow{\phi_\sigma} & \mathbb{C}^{|\Sigma(1)|} \setminus Z(\Sigma) \\ \downarrow & & \downarrow \\ U_\sigma & \hookrightarrow & X_\Sigma \end{array}$$

where vertical arrows are the maps from the quotient construction and, since σ is smooth, the left one is an isomorphism.

This means that if a closed subvariety $Y \subset X_\Sigma$ is defined by an ideal $I \subseteq S$ (i.e. it is a quotient by G of a subvariety of $\operatorname{Spec}(S)$) then its local piece $U_\sigma \cap Y$ for a smooth cone σ is the zero set of $\widetilde{I} \subset \mathbb{C}[x_\rho \colon \rho \in \sigma(1)]$ obtained by setting $x_\rho = 1$ for all $\rho \notin \sigma(1)$.
However, we need to consider this situation in a more general case where σ is not necessarily smooth, but it is simplicial. Then U_σ is a quotient of an affine space by a finite abelian group action and we describe locally a subvariety of X_Σ given by $I \subset S$ not on U_σ, but on an affine space whose quotient is U_σ. Thus we can present $Y \cap U_\sigma$ as a quotient of an affine variety by a finite group action.

Proposition 2.2.7. *In the setting as above let $\sigma \in \Sigma$ be a simplicial cone of maximal dimension. Then the diagram from Proposition 2.2.6, where vertical arrows are the maps from the quotient construction, commutes. Moreover, the left vertical arrow is a quotient by an action of a finite group H, which is the cokernel of the lattice homomorphism $h \colon \mathbb{Z}^{|\sigma(1)|} \to N$ corresponding to this map.*

Proof. The argument for the commutativity of the diagram given in the proof of [CLS11, Prop. 5.2.10] works without changes also in this case.
The monomorphism $h \colon \mathbb{Z}^{|\sigma(1)|} \to N$ corresponding to the left vertical map takes an element e_ρ of the standard basis of $\mathbb{Z}^{|\sigma(1)|}$ to the ray ρ of σ. Since σ is of maximal dimension and simplicial, the set of its rays is a basis of $N_\mathbb{R}$. Thus the cokernel of h is a finite abelian group. It is isomorphic to the kernel of the dual homomorphism of lattices, hence also, by definition, to the group G from the quotient construction. □

The statement concerning the commutativity of the diagram as above is true in a more general setting. The left vertical map can be the morphism from quotient construction not only for a single cone, but for a subfan of Σ satisfying certain assumptions (see exercise 5.2.5 in [CLS11]). However, here only the version from Proposition 2.2.7 will be used.

2.3 Toric varieties from polytopes and normality

In the second part of the thesis (chapters 6-8) we consider toric varieties which appear as geometric models of phylogenetic trees with a finite group action. These varieties do not have to be normal, hence they do not necessarily come from a fan. However, the natural way of describing them is to construct a lattice polytope directly from the structure of the phylogenetic tree (see section 8.1.1). Therefore we recall the notation for presenting toric varieties in terms of lattice polytopes and we state a few properties which will be used to check normality and projective normality of such varieties.
Let P denote a **lattice polytope** in $M_{\mathbb{R}}$, that is a convex hull of a finite set of lattice points $S \subseteq M$. The set of lattice points inside P is $\{m_1, \dots, m_s\} = P \cap M$. Let $\dim M_{\mathbb{R}} = n$. Then $T_N \simeq (\mathbb{C}^*)^n$ and its points are denoted by $(t_1, \dots, t_n) \in T_N$. The Laurent monomial $\chi^v(t_1, \dots, t_n)$ is the character of T_N corresponding to $v \in M$.

Definition 2.3.1. By a **projective toric variety associated with a lattice polytope** $P \subset M_{\mathbb{R}}$ we understand the Zariski closure of the map

$$(t_1, \dots, t_n) \mapsto [\chi^{m_1}(t_1, \dots, t_n) : \dots : \chi^{m_s}(t_1, \dots, t_n)] \in \mathbb{P}^{s-1}$$

This variety will be denoted by X_P.

Note that this is slightly different from the construction in [CLS11, Ch. 2] in the case where X_P is not projectively normal. Also, we intentionally skip the relation between toric varieties constructed from polytopes and the representation by fans (see e.g. [CLS11, Sect. 2.3]), because it is not used explicitly throughout the text.

Definition 2.3.2. The **affine cone** over X_P, denoted by C_P, is the Zariski closure of the map

$$(t_1, \dots, t_n, z) \mapsto (\chi^{m_1}(t_1, \dots, t_n) \cdot z, \dots, \chi^{m_s}(t_1, \dots, t_n) \cdot z) \in \mathbb{C}^s,$$

where $(t_1, \dots, t_n, z) \in (\mathbb{C}^*)^s \times \mathbb{C}$. In other words, C_P is the spectrum of the semigroup generated by $(P \times \{1\}) \cap (M \times \mathbb{Z})$.

Lemma 2.3.3. *[Stu96, Lem. 4.1] The toric ideal $I_P \subseteq \mathbb{C}[x_1, \dots, x_s]$ associated with P, i.e. the ideal of C_P, is spanned ac a $\mathbb{C}$-vector space by the set of binomials*

$$x_1^{u_1} \cdots x_s^{u_s} - x_1^{v_1} \cdots x_s^{v_s}$$

such that there is a relation $\sum_{i=1}^{s} u_i(m_i \times \{1\}) = \sum_{i=1}^{s} v_i(m_i \times \{1\})$ between vertices of $P \times \{1\}$.

In chapter 8 we investigate normality of toric varieties constructed from lattice polytopes, so we recall necessary definitions and equivalent combinatorial conditions below.

Definition 2.3.4. An algebraic variety is **normal** if it can be covered by open affine subsets which are normal, that is their coordinate rings are integrally closed in their fields of fractions. A projective variety is **projectively normal** if the affine cone over it is a normal (affine) variety.

Definition 2.3.5. [CLS11, Lem. 2.2.14, Def 2.2.17] We will say that a lattice polytope $P \subseteq M_{\mathbb{R}}$ is **normal** if the set $(P \cap M) \times \{1\}$ generates the semigroup $\mathrm{Cone}(P \times \{1\}) \cap (M \times \mathbb{Z})$.
P will be called **very ample** if for every vertex m of P the semigroup $S_{P,m}$ generated by the set $P \cap M - m = \{m' - m \colon m' \in P \cap M\}$ is saturated in M, i.e. there are no $x \in M$ and $k \in \mathbb{N}$ such that $nx \in S_{P,m}$ and $x \notin S_{P,m}$.

Two useful facts in the lemma below follow directly from [CLS11, Thm 1.3.5] and Definition 2.3.5.

Lemma 2.3.6. *The projective variety X_P associated with a lattice polytope P is normal if and only if P is very ample. The affine cone C_P over X_P is normal, i.e. X_P is projectively normal, if and only if P is normal.*

Remark 2.3.7. Lattice polytopes considered in chapter 8 appear in a natural way lying in a hyperplane $H \subset M_{\mathbb{R}}$ given by a condition that the sum of a certain group of coordinates is one (for the details see section 8.1.1). Then, instead of considering such a polytope P in H and looking at the semigroup generated by lattice points of $P \times \{1\}$ in $H \times \mathbb{Z}$ we may think of the semigroup generated by lattice points of P in M, since there is the isomorphism of lattices $H \times \{1\} \to M$ mapping lattice points in $P \times \{1\}$ to lattice points in P. This fact will be used for checking normality and computing Hilbert-Ehrhart polynomials of certain varieties associated with polytopes in chapter 8. Note also, that in this case the toric ideal I_P is homogeneous.

Chapter 3

Singularities, resolutions, Cox rings

In this chapter the main objects investigated in this work are described. First of all, we give basic definitions and general results on quotient singularities and their resolutions. In section 3.2, we present the classification of 2-dimensional quotient singularities by saying how to construct corresponding subgroups of $GL(2, \mathbb{C})$ from basic components. We compute their commutator subgroups and abelianizations, needed in section 4.2.6 and chapter 5. Then minimal resolutions of these singularities are described. First the case of cyclic groups, which are toric, hence their Cox ring is just a polynomial ring; see section 3.3. Next, the resolutions of quotients by non-cyclic groups, which are investigated in what follows; see section 3.4. These three sections are based on works [Bri68] and [Rie77]. Finally, in section 3.5 a very brief introduction into the theory of Cox rings of algebraic varieties is provided.

3.1 Quotient singularities, resolutions

By a quotient singularity we understand a singular point x of a quotient X/G, where X is a smooth algebraic variety and G is a finite group action on X by algebraic automorphisms. They are locally analytically isomorphic to quotients of affine spaces by linear actions.

Theorem 3.1.1 (Cartan)**.** *Any complex quotient singularity $(X/G, x)$ is isomorphic to $(\mathbb{C}^n/G, 0)$, where $G \subset GL(n, \mathbb{C})$ is a finite subgroup.*

Therefore we investigate quotients of an affine space $V \simeq \mathbb{C}^n$ by linear actions of finite groups in the special case of $n = 2$. The quotient is just the spectrum of the ring of invariants of the action,

$$V/G = \operatorname{Spec}(\mathbb{C}[V]^G).$$

The definition of the quotient works because of the following old result of E. Noether.

Theorem 3.1.2 (Noether)**.** *The ring of polynomial invariants of a linear action of a finite group on an affine space is finitely generated.*

As the ring of invariants depends only on the conjugacy class of G, the quotients for conjugate groups are isomorphic. Hence we consider only a representative for each (interesting) conjugacy class.

Definition 3.1.3. A **pseudo-reflection** (or a quasi-reflection) is a linear transformation of dimension n which has 1 as an eigenvalue with multiplicity $n-1$.

The Chevalley-Shephard-Todd theorem (see e.g. [Stu93, Section 2.4]) states that the ring of invariants of a finite linear group action is a polynomial ring if and only if the group is generated by pseudo-reflections. In other words, a finite group G generated by pseudo-reflections is not interesting in the context of our problem, because $V/G \simeq V$. For any finite $G \subset GL(n, \mathbb{C})$ the subgroup R generated by pseudo-reflections is normal, G/R does not contain pseudo-reflections and, due to this result, $V/G \simeq V/(G/R)$. Therefore, we can restrict ourselves to considering (conjugacy classes of) small groups.

Definition 3.1.4. A subgroup of $GL(n, \mathbb{C})$ is a **small group** if it does not contain any pseudo-reflection.

The quotient of $\mathbb{C}^2$ by a finite subgroup of $G \subset GL(2, \mathbb{C})$ either is smooth or has an isolated singularity in 0. This is because if a non-zero point has a non-trivial isotropy group H, then every element of H has an eigenvalue 1, so it is a pseudo-reflection. However, it is worth noting that in higher dimensions the singular locus of a quotient of an affine space by a finite linear group action can be much more complicated.
We sum up the discussion in the following definition.

Definition 3.1.5. We use the term (complex) **surface quotient singularity** for a quotient of $\mathbb{C}^2$ by a linear action of a finite small group G. This variety is normal, singular at 0 and smooth in all other points.

In section 3.2 we describe the classification of finite small subgroups of $GL(2, \mathbb{C})$, hence also the classification of surface quotient singularities up to isomorphism.
We now state the basic properties of the resolution of singularities of finite quotients in dimension 2.

Definition 3.1.6. A smooth variety Y is a **resolution of singularities** of a normal variety X if there is a proper birational morphism $f\colon Y \to X$ such that it restricts to an isomorphism $Y \setminus f^{-1}(Sing(X)) \xrightarrow{\simeq} X \setminus Sing(X)$.

Definition 3.1.7. The **exceptional set** of a resolution $f\colon Y \to X$ is $f^{-1}(Sing(X))$. In case of resolutions of surface quotient singularities $\mathbb{C}^2/G$ it is just $f^{-1}(0)$ and it has codimension one in Y, so we use the term **exceptional divisor**.

Definition 3.1.8. The **minimal resolution of singularities** of a surface X is a resolution $f\colon Y \to X$ such that every other resolution $f'\colon Y' \to X$ factors through $\varphi\colon Y' \to Y$.
In case of resolutions of isolated surface singularities it is equivalent to a statement that the exceptional divisor does not contain (-1)-curves.

In general, the minimal resolution does not necessarily exist, but in dimension 2 it does.
Quotient singularities are rational, see e.g. [Bri68] for the surface case and [Bur74, Vie77] for higher dimensional cases. The exceptional divisor of a resolution of a rational surface singularity has the following properties (see [Bri68, Lem. 1.3]):

- its irreducible components are smooth rational curves, which form a tree (i.e. an acyclic graph),
- two different irreducible components intersect in at most one point, and if they do, their intersection number is 1,
- no three irreducible components intersect.

We will see in section 3.4 that in case of surface quotient singularities the exceptional fibre is a very simple tree of $\mathbb{P}^1$ curves. It can be either a chain or a tree consisting of three chains joined in a central component – its dual graph is a so-called T-shaped diagram, as in Fig. 3.2. The details, in particular the self-intersection numbers of components, are given in section 3.4.

3.2 Finite small subgroups of $GL(2, \mathbb{C})$

This section contains the list of groups for which we consider the quotient singularity $\mathbb{C}^2/G$. We also compute commutator subgroups and abelianizations of considered groups, which will be needed in the sequel, especially in section 5.2.
The classification of (conjugacy classes of) finite small subgroups of $GL(2, \mathbb{C})$ is taken from [Bri68] and [Rie77]. Before listing the groups we introduce the notation for the cases which are constructed via fibre product (after [Bri68]).
By $\mu\colon GL(2, \mathbb{C}) \times GL(2, \mathbb{C}) \to GL(2, \mathbb{C})$ we denote the matrix multiplication.

Definition 3.2.1. Take $H_1, H_2 \subset GL(2, \mathbb{C})$ with normal subgroups N_1 and N_2 respectively, such that there is an isomorphism $\phi : H_1/N_1 \to H_2/N_2$. By $[h_i]$ we denote the class of $h_i \in H_i$ in H_i/N_i. We will consider the image under μ of the fibre product of H_1 and H_2 over ϕ:

$$(H_1, N_1; H_2, N_2)_\phi = \mu(\{(h_1, h_2) \in H_1 \times H_2 \colon [h_2] = \phi([h_1])\}).$$

If the choice of ϕ is obvious, it will be denoted by $(H_1, N_1; H_2, N_2)$.

Throughout the text we use the usual notation $\varepsilon_n = e^{2\pi i/n}$.

Proposition 3.2.2. [Bri68, Satz 2.9] *The conjugacy classes of finite small subgroups of $GL(2, \mathbb{C})$ are:*

1. *cyclic groups $C_{n,q} = \langle \mathrm{diag}(\varepsilon_n, \varepsilon_n^q) \rangle$, where $C_{n,q}$ is conjugate to $C_{n,q'}$ if and only if $q = q'$ or $qq' \equiv 1 \mod n$,*
2. *non-cyclic groups contained in $SL(2, \mathbb{C})$:*

- *binary dihedral groups BD_n ($4n$ elements, $n \geq 2$, gives the Du Val singularity D_{n+2}),*
- *binary tetrahedral group BT (24 elements, Du Val singularity E_6),*
- *binary octahedral group BO (48 elements, Du Val singularity E_7),*
- *binary icosahedral group BI (120 elements, Du Val singularity E_8),*

3. *images under μ of fibre products of a group in $SL(2,\mathbb{C})$ and a cyclic group $Z_k = C_{k,1} = \mathrm{diag}(\varepsilon_k, \varepsilon_k)$ contained in the center of $GL(2,\mathbb{C})$:*

    - *$BD_{n,m}$ for $(m,n) = 1$, defined as $(Z_{2m}, Z_{2m}; BD_n, BD_n)$ for odd m and $(Z_{4m}, Z_{2m}; BD_n, C_{2n})$, where $C_{2n} \lhd BD_n$ is cyclic of order $2n$, when m is even,*
    - *BT_m defined as $(Z_{2m}, Z_{2m}; BT, BT)$ in the cases where $(m,6) = 1$ and as $(Z_{6m}, Z_{2m}; BT, BD_2)$ when $(m,6) = 3$,*
    - *$BO_m = (Z_{2m}, Z_{2m}; BO, BO)$ if $(m,6) = 1$,*
    - *$BI_m = (Z_{2m}, Z_{2m}; BI, BI)$ if $(m,30) = 1$.*

    Note that for $m = 1$ we obtain the subgroups of $SL(2,\mathbb{C})$ listed above.

In what follows, by abuse of notation, we most often identify the conjugacy classes of subgroups of $GL(2,\mathbb{C})$ and their representatives from the list in Proposition 3.2.2. Generators of each of these groups can be found in [Rie77]. However, we intend to avoid lengthy computations using generators, hence we do not list them here. We need only the description of abelianizations of considered groups in terms of generating sets, given in Corollary 3.2.5.
Quotients by cyclic groups are toric singularities. The structure of their Cox rings, which are just polynomial rings, is well known. We provide some information on this case in section 3.3 based on [CLS11, Chapter 5]) and in what follows we consider only quotients by non-cyclic groups.
Generators of finite small subgroups of $SL(2,\mathbb{C})$ are given e.g. in [Rei]. A simple computation, performed for example in [GAP12], allows to prove the following lemma.

Lemma 3.2.3. *The commutator subgroups and the abelianizations of finite small subgroups of $SL(2,\mathbb{C})$ are:*

- *$[BD_n, BD_n] \simeq \mathbb{Z}_n$, it is generated by $\mathrm{diag}(\varepsilon_n, \varepsilon_n^{-1})$, $Ab(BD_n)$ is $\mathbb{Z}_2 \times \mathbb{Z}_2$ if n is even and $\mathbb{Z}_4$ for odd n,*
- *$[BT, BT] = BD_2$, $Ab(BT) \simeq \mathbb{Z}_3$,*
- *$[BO, BO] = BT$, $Ab(BO) \simeq \mathbb{Z}_2$,*
- *$[BI, BI] = BI$, $Ab(BI) = 1$.*

It turns out that commutator subgroups of finite small subgroups of $GL(2,\mathbb{C})$ are the same as for $SL(2,\mathbb{C})$ subgroups.

Lemma 3.2.4. *The commutator subgroup of a small subgroup $G \subset GL(2,\mathbb{C})$ from the list in Proposition 3.2.2 (3) is the same as the commutator subgroup of the non-cyclic factor of the corresponding fibre product structure given in Proposition 3.2.2.*

Proof. Let $G = (H_1, N_1; H_2, N_2)$ such that H_1 is in the center of $GL(2,\mathbb{C})$. Take $g, g' \in G$ and let $g = h_1h_2$, $g' = h_1'h_2'$ where $h_i, h_i' \in H_i$. Then $gg'g^{-1}g'^{-1} = h_2h_2'h_2^{-1}h_2'^{-1}$, so $[G,G] \subseteq [H_2,H_2]$. They are equal, since by Definition 3.2.1 for every $h_2 \in H_2$ there exists some $h_1 \in H_1$ such that $h_1h_2 \in G$. $\square$

Now the abelianizations of considered groups can be computed. In fact, if we needed only their isomorphism types, we could read them out from the last column of the table in [Bri68, p. 348]. (This is because $Ab(G)$ of $G \subset GL(n,\mathbb{C})$ is isomorphic to the class group of the quotient variety $\mathbb{C}^n/G$, see Proposition 3.4.8.) However, the proof of Proposition 4.2.10 requires knowing generators of $Ab(G)$, hence we list them below. They are written as matrices in $GL(2,\mathbb{C})$ whose classes generate $G/[G,G]$. To describe generators of $Ab(G)$ we use

$$B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \text{and} \qquad C = \frac{1}{2}\begin{pmatrix} 1+i & -1+i \\ 1+i & 1-i \end{pmatrix}.$$

Corollary 3.2.5. *Abelianizations of finite small subgroups of $GL(2,\mathbb{C})$ are*

- *if n is even, $Ab(BD_{n,m}) \simeq \mathbb{Z}_{2m} \times \mathbb{Z}_2$ is generated by $\varepsilon_{2m} \cdot B$ and $\mathrm{diag}(\varepsilon_{2n}, \varepsilon_{2n}^{-1})$,*
- *if n is odd, $Ab(BD_{n,m}) \simeq \mathbb{Z}_{4m}$ is generated by $\varepsilon_{4m} \cdot B$ for m even and $\varepsilon_{2m} \cdot B$ for m odd,*
- *$Ab(BT_m) \simeq \mathbb{Z}_{3m}$ is generated by*
  - ⋆ *$\varepsilon_{2m} \cdot C$ if $(m,6) = 1$,*
  - ⋆ *$\varepsilon_{6m} \cdot C$ if $(m,6) = 3$,*
- *$Ab(BO_m) \simeq \mathbb{Z}_{2m}$ is generated by $\varepsilon_{2m} \cdot \mathrm{diag}(\varepsilon_8, \varepsilon_8^{-1})$,*
- *$Ab(BI_m) \simeq \mathbb{Z}_m$ is generated by $\mathrm{diag}(\varepsilon_m, \varepsilon_m)$.*

Proof. Assume $G = (H_1, N_1; H_2, N_2)$, where H_1 is a cyclic group generated by $\mathrm{diag}(\varepsilon_{2k}, \varepsilon_{2k})$ and H_2 a subgroup of $SL(2,\mathbb{C})$.
We start from computing the order of $Ab(G)$. The order of $[G,G]$ is known by Lemma 3.2.3, so we only have to determine the order of G. Look at the kernel of

$$\mu\colon \{(h_1,h_2) \in H_1 \times H_2 \colon [h_2] = \phi([h_1])\} \to GL(2,\mathbb{C}).$$

Take $0 < i \leq 2k$ and $M \in SL(2,\mathbb{C})$ such that $\varepsilon_{2k}^i \cdot M = 1$. Then $\mathrm{diag}(\varepsilon_{2k}^{-i}, \varepsilon_{2k}^{-i})$ is in $SL(2,\mathbb{C})$, which is possible only if $i = k$ or $i = 2k$, i.e. $M = \mathrm{diag}(-1,-1)$ or $M = \mathrm{diag}(\varepsilon_{2k}^{-2k}, \varepsilon_{2k}^{-2k}) = 1$. Since for any considered group G both these pairs of matrices are in the fibre product (which can be checked directly using the list in Proposition 3.2.2), the kernel is always $\mathbb{Z}_2$. Thus

$$|Ab(G)| = |G|/|[G,G]| = |N_1| \cdot |N_2| \cdot (|H_1|/|N_1|)/(|\ker \mu| \cdot |[G,G]|) = \\ = |H_1| \cdot |N_2|/(2|[G,G]|).$$

We check case by case that the values obtained this way are compatible with the formulation of this corollary.
Now in all cases but the first one it suffices to say that the order of the element given in the formulation of the corollary modulo $[G,G]$ is in fact equal to the order of $Ab(G)$. For example take the case of $G = BD_{n,m}$ for odd n. If m is even then $G = (Z_{4m}, Z_{2m}; BD_n, C_{2n})$ and $\varepsilon_{4m} \cdot B \in G$. Assume $(\varepsilon_{4m} \cdot B)^a \in [G,G] \subset SL(2,\mathbb{C})$ for some $0 < a < 4m$. The determinant of this element is ε_{4m}^{2a}, so $a = 2m$. But then $2m$ is a multiple of 4 and $\varepsilon_{4m}^{2m} \cdot B^{2m} = \mathrm{diag}(-1,-1)$, which is not in $[G,G] \simeq \mathbb{Z}_n$, because n is odd. Thus $\varepsilon_{4m} \cdot B$ is indeed of order $4m$. If m is also odd then $G = (Z_{2m}, Z_{2m}; BD_n, BD_n)$ and from $(\varepsilon_{2m} \cdot B)^a \in [G,G] \subset SL(2,\mathbb{C})$ we have $a = m$. But $(\varepsilon_{2m} \cdot B)^m$ is $i \cdot B$ or $i \cdot B^{-1}$, which is not diagonal, hence it is not in $[G,G]$. The remaining cyclic cases can be checked in the same way.
In the case of $G = BD_{n,m}$ for n even the number m must be odd, so we have $G = (Z_{2m}, Z_{2m}; BD_n, BD_n)$. As before, $\varepsilon_{2m} \cdot B$ is of order $2m$, and $\mathrm{diag}(\varepsilon_{2n}, \varepsilon_{2n}^{-1})$ has order 2 modulo $[G,G]$. The commutator of these elements is $\mathrm{diag}(\varepsilon_{2n}^{-2}, \varepsilon_{2n}^{2})$, so it is in $[G,G] \simeq \mathbb{Z}_n = \langle(\mathrm{diag}(\varepsilon_{2n}, \varepsilon_{2n}^{-1}))^2\rangle$ and chosen elements represent commutative classes of $Ab(G)$. Moreover, $(\varepsilon_{2m} \cdot B)^m = -B^m$ and $-B^m \cdot \mathrm{diag}(\varepsilon_{2n}, \varepsilon_{2n}^{-1}) \notin [G,G]$, so the element of order 2 is not in the subgroup generated by $\varepsilon_{2m} \cdot B$. Thus in fact $Ab(G) \simeq \mathbb{Z}_{2m} \times \mathbb{Z}_2$. □

3.3 Cyclic quotient singularities: resolutions and Cox rings

Before we consider minimal resolutions of surface quotient singularities in general, we summarize briefly the case of quotients by abelian finite small subgroups of $GL(2,\mathbb{C})$, i.e. cyclic groups. Then the singularity and its minimal resolutions are toric. Hence their total coordinate ring can be described without giving a more general definition than what we have stated in 2.2.5. Moreover, this case gives an opportunity for defining a few objects which reappear in the description of the minimal resolutions in non-cyclic cases. The main sources for this section are [Ful93, Sect. 2.2, Sect. 2.6] and [Rei97].
Let $G = C_{n,q} = \langle \mathrm{diag}(\varepsilon_n, \varepsilon_n^q)\rangle$ where $\varepsilon_n = e^{2\pi i/n}$ and $(n,q) = 1$. In the notation of [Rei97] it is $\frac{1}{n}(1,q)$. We consider the action of G on $\mathbb{C}^2$ and the quotient singularity $\mathbb{C}^2/G$.

Remark 3.3.1. [Ful93, Sect. 2.2] The quotient $\mathbb{C}^2/G$ has a toric structure. Let e_1, e_2 be the standard basis of $N \simeq \mathbb{Z}^2$. The fan of $\mathbb{C}^2/G$ consists of a single 2-dimensional cone $\sigma_{n,q} \subset N_{\mathbb{R}} \simeq \mathbb{R}^2$ (and all its faces) spanned by $ne_1 - qe_2$ and e_2.

Its minimal resolution can also be described in the toric setting. Its fan is obtained by dividing $\sigma_{n,q}$ into subcones by some carefully chosen rays. We sketch the construction explained in more detail in [Ful93, Sect. 2.6].

Construction 3.3.2. We construct the set of rays which divide $\sigma_{n,q}$ into smooth cones recursively.

1. The subcone of $\sigma_{n,q}$ spanned by e_1 and e_2 is smooth, so draw the ray $\mathrm{Cone}(e_1)$ and then deal with the singularity of $\mathrm{Cone}(e_1, ne_1 - qe_2)$.

2. Find a cone $\sigma_{n',q'}$ such that there is a lattice automorphism of N mapping $\mathrm{Cone}(e_1, ne_1 - qe_2)$ to it: take $n' = q$ and $q' = a'q - n$ for some integer a' such that $0 \leq q' < n'$.

3. If $q' \neq 0$, then resolve the singularity of $\sigma_{n',q'}$.

Since in the second step both parameters decrease, the process stops. Because it started with n, q relatively prime, at the end we get $\sigma_{n',q'} = \mathrm{Cone}(e_1, e_2)$. By reversing all the chosen automorphisms we obtain the division of $\sigma_{n,q}$.

Example 3.3.3. Consider $\mathbb{C}^2/G$ where $G = C_{5,2} = \langle \mathrm{diag}(\varepsilon_5, \varepsilon_5^2)\rangle \simeq \mathbb{Z}_5$. This quotient corresponds to the cone $\sigma_{5,2}$ spanned by $e_2 = (0, 1)$ and $(5, -2)$, in the left part of Fig. 3.1. We divide this cone with vector $e_1 = (1, 0)$ into $\mathrm{Cone}(e_1, e_2)$, which is smooth (the light gray cone in the middle part of Fig. 3.1), and $\mathrm{Cone}(e_1, (5, -2))$, which is singular (the dark gray cone). The automorphism of $N \simeq \mathbb{Z}_2$ given by $\begin{pmatrix} 0 & -1 \\ 1 & 3 \end{pmatrix}$ maps the latter cone to $\sigma_{n',q'} = \sigma_{2,1} = \mathrm{Cone}(e_2, (2, -1))$, in particular $a' = 3$.

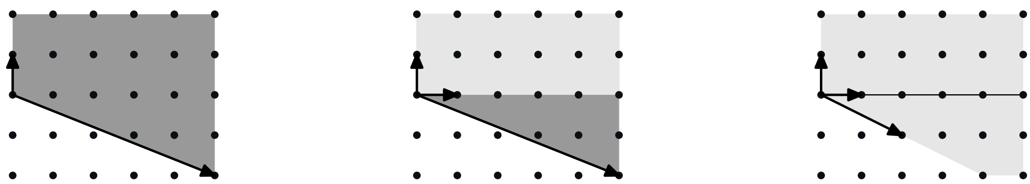


Figure 3.1: Steps of construction of the toric resolution of $\mathbb{C}^2/C_{2,5}$

When we divide $\sigma_{2,1}$ with e_1, we obtain two smooth cones, as in the right part of Fig. 3.1. More precisely, $\mathrm{Cone}(e_1, (2, -1))$ can be mapped to the positive quadrant of $N_{\mathbb{R}}$ by an automorphism $\begin{pmatrix} 0 & -1 \\ 1 & 2 \end{pmatrix}$, i.e. in this step $a' = 2$.

Definition 3.3.4. Let $0 < q < n$ be coprime integers. Then the Hirzebruch-Jung continued fraction is an expression

$$\frac{n}{q} = a_1 - \frac{1}{a_2 - \frac{1}{\dots - \frac{1}{a_m}}} = [a_1, a_2, \dots, a_m].$$

Corollary 3.3.5. *The sequence $[a_1, a_2, \dots, a_m]$ of values of the parameter a' obtained while performing the algorithm for $\sigma_{n,q}$ is exactly the resolution of the fraction n/q into the Hirzebruch-Jung continued fraction.*

Example 3.3.6. In the case of $G = C_{5,2} = \langle \mathrm{diag}(\varepsilon_5, \varepsilon_5^2)\rangle$ from Example 3.3.3 the sequence of values taken by the parameter a' is $[3, 2]$, which corresponds to the Hirzebruch-Jung continued fraction $5/2 = 3 - 1/2$.

Remark 3.3.7. It follows from the orbit-cone correspondence theorem (see [CLS11, Thm. 3.2.6]) that the exceptional divisor of the minimal resolution of $\mathbb{C}^2/G$ is the chain of $\mathbb{P}^1$ curves, intersecting each other transversally, of length m. A simple computation of the intersection product in the toric setting (see e.g. [CLS11, Sect. 6.3]) shows that their self-intersection numbers are $-a_1, -a_2, \dots, -a_m$.

Look at a matrix A determined by the entries of Hirzebruch-Jung continued fraction for n/q:

$$A = \begin{pmatrix} 1 & -a_1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -a_2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -a_3 & 1 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 1 & -a_{m-1} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -a_m & 1 \end{pmatrix}.$$

One can obtain two vectors $\alpha = (\alpha_0, \dots, \alpha_{m+1})$ and $\beta = (\beta_0, \dots, \beta_{m+1})$ in the kernel of the linear map given by A by taking the first two entries to be $\alpha_0 = 1$, $\alpha_1 = 0$ and $\beta_0 = 0$, $\beta_1 = 1$, and computing directly the remaining ones. By checking that the relations between entries are exactly the same as the relations between consecutive rays of the fan $\Sigma_{n,q}$ of the resolution in Construction 3.3.5, we get the following result.

Proposition 3.3.8. *The matrix K composed of two rows α and β defines a lattice epimorphism $\mathbb{Z}^{|\Sigma_{n,q}(1)|} \simeq \mathbb{Z}^{m+2} \to N \simeq \mathbb{Z}^2$ associated with the toric morphism*

$$\pi\colon \mathbb{C}^{|\Sigma_{n,q}(1)|} \setminus Z(\Sigma_{n,q}) \to U_{\sigma_{n,q}}$$

from the quotient construction (Theorem 2.2.4). Therefore K^t and A give the linear maps in the exact sequence of dual lattices (in some chosen coordinates)

$$0 \longrightarrow M \xrightarrow{K^t} \mathrm{Div}_{T_N}(X_\Sigma) \xrightarrow{A} \mathrm{Cl}(X_{\Sigma_{n,q}}) \longrightarrow 0.$$

Remark 3.3.9. It follows that A^t defines the map

$$\mathrm{Hom}_{\mathbb{Z}}(\mathrm{Cl}(X_{\Sigma_{n,q}}), \mathbb{C}^*) \longrightarrow (\mathbb{C}^*)^{|\Sigma_{n,q}(1)|}$$

which is an embedding of the group from the quotient construction onto a subtorus of the torus of $\mathbb{C}^{\Sigma(1)}$.

By Remark 2.2.5 the latter space is the spectrum of the total coordinate ring of the minimal resolution $X_{\Sigma_{n,q}}$ of $U_{\sigma_{n,q}}$. Therefore the quotient construction is just dividing the spectrum of the total coordinate ring of the resolution by a subtorus of its torus, defined by a formula depending on the intersection numbers of the components of the exceptional fibre. We will attempt to apply a similar procedure in the cases of non-toric quotient singularities.

3.4 Resolutions for $G < GL(2, \mathbb{C})$

The aim of this section is to describe precisely the exceptional divisors of minimal resolutions of surface quotient singularities $\mathbb{C}^2/G$ for non-cyclic groups. In this case irreducible components are smooth $\mathbb{P}^1$ curves forming a simple tree consisting of a central components with three chains attached, as in Fig. 3.2. We present the exceptional divisor of the resolutions by drawing their dual graphs: vertices correspond to irreducible components, edges to their intersection points, numbers are self-intersection numbers of components. At the end of the section we describe the Picard group and the class group (of Weil divisors) of $\mathbb{C}^2/G$ and of its minimal resolution. The material presented here is known, see e.g. [Bri68, Rie77].

3.4.1 Exceptional divisor

For quotients by subgroups of $SL(2, \mathbb{C})$ the dual graphs are just Dynkin diagrams of the root systems D_n for $n \geq 4$, E_6, E_7 and E_8. In this case all rational curves in the exceptional fibre have self-intersection -2. For the groups not contained in $SL(2, \mathbb{C})$ the diagrams do not have to be Dynkin diagrams any more, and also the self-intersection numbers can be less then -2, as it is shown in Examples 3.4.3 and 3.4.4. The structure of exceptional fibres for small subgroups of $GL(2, \mathbb{C})$ is described in details for example in [Bri68] and [Rie77]. Based on these works we list here a few properties needed in the further part of this text. We start from fixing the notation.
Let G be a finite small subgroup $G \subset GL(2, \mathbb{C})$. By X we denote the minimal resolution of the quotient singularity $\mathbb{C}^2/G$. We describe the exceptional divisor of the resolution morphism $X \to \mathbb{C}^2/G$ and its dual graph.

Notation 3.4.1. Let E_0 be the curve corresponding to the branching point of the diagram and $E_{i,j}$ be the j-th curve in the i-th branch, counting from E_0, as in Fig. 3.2.
If we need to write components of the exceptional divisor in a sequence, we always order them as follows:

$$E_0; E_{1,1}, \ldots, E_{1,n_1}; E_{2,1}, \ldots, E_{2,n_2}; E_{3,1}, \ldots, E_{3,n_3}.$$

The number of components of the exceptional divisor is $n = n_1 + n_2 + n_3 + 1$.
We will assume that $n_1 \leq n_2 \leq n_3$.

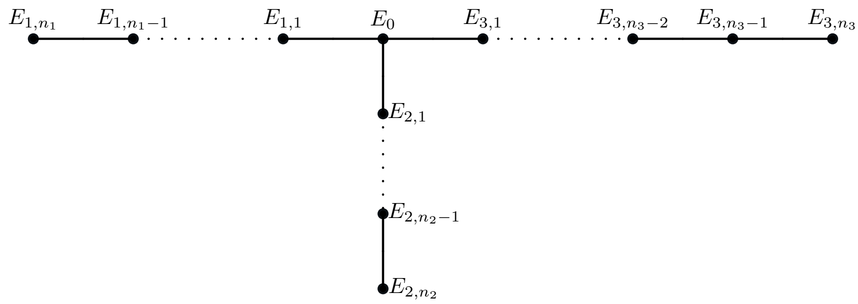


Figure 3.2: Dual graph of the exceptional divisor of the minimal resolution of $\mathbb{C}^2/G$

At the end of section 3.1 we remarked that $E_{i,j} \cdot E_{k,l} = 1$ (and $E_0 \cdot E_{i,j} = 1$) if these curves are adjacent and 0 if they are different and not adjacent. Hence we only have to describe the self-intersection numbers $E_{i,j} \cdot E_{i,j}$ and $E_0 \cdot E_0$.

Definition 3.4.2. We will denote by

$$\langle d;\ p_1, q_1;\ p_2, q_2;\ p_3, q_3 \rangle,$$

an invariant consisting of seven integers, which contains full information about the intersection numbers of components of the exceptional divisor of the minimal resolution of $\mathbb{C}^2/G$ for a non-cyclic small group $G \subset GL(2, \mathbb{C})$. We will be using the following information:

- $d = -E_0 \cdot E_0$,
- the j-th entry of the expansion of p_i/q_i into the Hirzebruch-Jung continued fraction is equal to $-E_{i,j} \cdot E_{i,j}$ (hence the length of a branch is the length of the corresponding continued fraction),
- the exact rule how to restore these numbers from the group structure description can be found in [Bri68, Satz 2.11].

Broadly speaking, these numbers are connected to the fibre product description of the group structure (see Proposition 3.2.2). This follows from the construction of the resolution of $\mathbb{C}^2/G$ based on the well-understood minimal resolutions for the subgroups of $SL(2, \mathbb{C})$; for the details we refer the reader to [Bri68].

Example 3.4.3 (Quotients by $BD_{2,m}$)**.** The simplest case is $BD_{2,1} = BD_2 \subset SL(2, \mathbb{C})$, which gives the Du Val singularity D_4, whose dual graph has three branches of length 1 (see Fig. 3.3). As $(m, n) = 1$, other cases are $(\mathbb{Z}_{2m}, \mathbb{Z}_{2m}; BD_2, BD_2)$ where m is odd. Using the notation of [Bri68, Satz 2.11], the minimal resolution for $BD_{2,m}$ is described by the sequence $\langle -\frac{m+3}{2};\ 2, 1;\ 2, 1;\ 2, 1 \rangle$. Thus it turns out that the dual graphs of these resolutions are the same as for BD_2, but the self-intersection number in the branching point changes: for $BD_{2,m}$ it is $-\frac{m+3}{2}$.

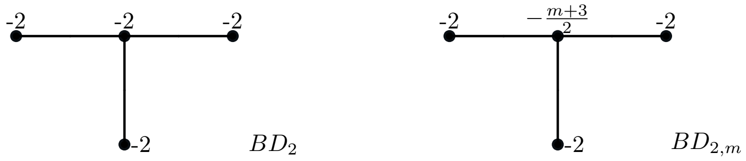


Figure 3.3: Dual graphs of exceptional divisors of minimal resolutions of $\mathbb{C}^2/BD_2$ and $\mathbb{C}^2/BD_{2,m}$

Example 3.4.4. Starting from larger binary dihedral groups and taking the fibre product with a suitable cyclic group one can obtain resolutions much different from the Du Val case. For example, for $BD_{23,39}$ the minimal resolution is described by the sequence $\langle d;\ 2,1;\ 2,1;\ 23,q\rangle$, where, according to the rule in [Bri68, Satz 2.11], $39 = 23(d-1) - q$. Thus $d = 3$ and $q = 7$, the continued fraction describing the last branch is

$$\frac{23}{7} = 4 - \frac{1}{2 - \frac{1}{2-\frac{1}{3}}}$$

and the dual graph (much smaller than the one for BD_{23}) is as in Fig. 3.4.

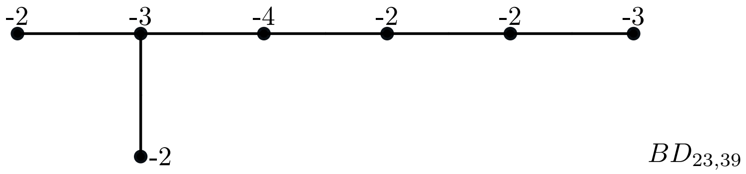


Figure 3.4: Dual graph of exceptional divisors of minimal resolution of $\mathbb{C}^2/BD_{23,39}$

Based on the intersection numbers of components of the exceptional divisor of the minimal resolution we define a matrix U which will be called an **extended intersection matrix** for the singularity $\mathbb{C}^2/G$.

We start from the intersection matrix U^0 of the components of the exceptional divisor. The curves are ordered as stated in Notation 3.4.1, so $U^0_{k,l}$ is the intersection number of the k-th and l-th curve in the sequence. We extend U^0 to a matrix U by adding three columns. One can imagine that to the ending curve of each branch we add a leaf – a curve which intersect (transversally) the last curve in a branch, but which is not an element of the exceptional fibre, so we do not include its self-intersection number. Hence, for $i = 1, 2, 3$, just after the column corresponding to E_{i,n_i}, we add a column filled with 0 except of the entry corresponding to E_{i,n_i}, where we put 1. (In fact, adding these columns corresponds to choosing three rational functions on $\mathbb{C}^2/G$, which are elements of the Cox ring of the singularity itself, and including them in a generating set of the Cox ring of the minimal resolutions. This attitude will be used and explained in detail in chapter 5.2.)

This construction will be used to define an action of a torus on the (candidate for the) spectrum of the Cox ring of the minimal resolution, which will be introduced in section 4.1.

Notation 3.4.5. Throughout the text we think of U as if it was divided in a few blocks:

$$\left(\begin{array}{c|cccc|c|cccc|c|cccc|c}
-d & 1 & 0 & \dots & 0 & 0 & 1 & 0 & \dots & 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ \hline
1 & & & & & 0 & & & & & & & & & & \\
0 & & & & & \vdots & & & & & & & & & & \\
\vdots & & A_1 & & & 0 & & 0 & & & 0 & & 0 & & & 0 \\
0 & & & & & 1 & & & & & & & & & & \\ \hline
1 & & & & & & & & & & 0 & & & & & \\
0 & & & & & & & & & & \vdots & & & & & \\
\vdots & & 0 & & & 0 & & A_2 & & & 0 & & 0 & & & 0 \\
0 & & & & & & & & & & 1 & & & & & \\ \hline
1 & & & & & & & & & & & & & & & 0 \\
0 & & & & & & & & & & & & & & & \vdots \\
\vdots & & 0 & & & 0 & & 0 & & & 0 & & A_3 & & & 0 \\
0 & & & & & & & & & & & & & & & 1
\end{array}\right)$$

The block denoted by A_i is the matrix of intersection numbers of components in the i-th branch of the exceptional divisor:

$$A_i = \begin{pmatrix}
-a_{i,1} & 1 & 0 & 0 & 0 & 0 \\
1 & -a_{i,2} & 1 & 0 & 0 & 0 \\
0 & 1 & -a_{i,3} & 1 & 0 & 0 \\
\dots & \dots & \dots & \dots & \dots & \dots \\
0 & 0 & 0 & 1 & -a_{i,n_i-1} & 1 \\
0 & 0 & 0 & 0 & 1 & -a_{i,n_i}
\end{pmatrix}$$

On the diagonal of A_i there is the sequence of the negatives of entries of the Hirzebruch-Jung continued fraction associated with the i-th branch of the exceptional divisor.

Remark 3.4.6. By Remark 3.3.7 the entries of A_i are the intersection numbers of the components of the exceptional divisor in the minimal resolution of the cyclic quotient singularity $\mathbb{C}^2/C_{p_i,q_i}$. Hence if we construct a matrix A_i' by adding columns $(1,0,\dots,0)^t$ and $(0,\dots,0,1)^t$ at the beginning and at the end of A_i, then $(A_i')^t$ determines the group from the toric quotient construction of the minimal resolution of $\mathbb{C}^2/C_{p_i,q_i}$, as described in Proposition 3.3.8. Cyclic quotient singularities $\mathbb{C}^2/C_{p_i,q_i}$ associated with $\mathbb{C}^2/G$ will appear later in the description of toric embedding of the minimal resolution in section 4.1.2.

In fact, results of Brieskorn give more restrictions for the description of the exceptional divisor of the minimal resolution. In particular, not all T-shaped diagrams can appear as dual graphs of the exceptional divisor. It turns out that one branch always has length one and also the second one cannot be too long. Moreover, there are restrictions for the self-intersection numbers of components (remember that $n_1 \leq n_2 \leq n_3$).

Remark 3.4.7. According to [Bri68, p. 348],

- $A_1 = (-2)$, i.e. $n_1 = 1$,
- at least one of A_2, A_3 is one of (-2), $\begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix}$, (-3),
- A_3 can be of any size only if $A_1 = A_2 = (-2)$; otherwise A_3 is at most 5×5 matrix.

3.4.2 The Picard group, the class group

We finish with a description of the Picard group and the class group of a quotient singularity and its minimal resolution.

Proposition 3.4.8. *For the singularity $\mathbb{C}^2/G$ we have*

$$\mathrm{Pic}(\mathbb{C}^2/G) = 0, \qquad \mathrm{Cl}(\mathbb{C}^2/G) \simeq Ab(G).$$

Proof. These two properties are Theorems 3.6.1 and 3.9.2 in [Ben93]. □

Proposition 3.4.9. *The Picard group of the minimal resolution X of $\mathbb{C}^2/G$ is a free abelian group generated by divisors dual to irreducible curves in the special fibre of this resolution. That is, if n is the number of exceptional curves of the minimal resolution, then*

$$\mathrm{Pic}(X) = \mathrm{Cl}(X) \simeq \mathbb{Z}^n.$$

Proof. Since X is smooth, $\mathrm{Cl}(X) = \mathrm{Pic}(X)$. We start from showing that $\mathrm{Pic}(X)$ is a lattice. First note that $H^1(X, \mathcal{O}_X) = H^2(X, \mathcal{O}_X) = 0$ because of rationality of $\mathbb{C}^2/G$. Then from the exponential sequence

$$\ldots \longrightarrow H^1(X, \mathcal{O}_X) \longrightarrow H^1(X, \mathcal{O}^*(X)) \longrightarrow H^2(X, \mathbb{Z}) \longrightarrow H^2(X, \mathcal{O}_X) \longrightarrow \ldots$$

we deduce that $\mathrm{Pic}(X) \simeq H^2(X, \mathbb{Z})$. By the universal coefficient theorem we have a short exact sequence

$$0 \longrightarrow \mathrm{Ext}(H_1(X, \mathbb{Z}), \mathbb{Z}) \longrightarrow H^2(X, \mathbb{Z}) \longrightarrow \mathrm{Hom}(H_2(X, \mathbb{Z}), \mathbb{Z}) \longrightarrow 0.$$

Its first term is 0, because $\pi_1(X)$ is trivial (the quotient space $\mathbb{C}^2/G$ is contractible and by [Kol93, Thm. 7.8] the blow-ups do not change the fundamental group). Thus $\mathrm{Pic}(X) \simeq \mathrm{Hom}(H_2(X, \mathbb{Z}), \mathbb{Z})$, which is torsion-free.
Because X can be contracted to the exceptional divisor, which by the rationality of $\mathbb{C}^2/G$ is a tree of rational curves, $H_2(X, \mathbb{Z})$ is a lattice generated by classes of exceptional curves. Thus $\mathrm{Pic}(X)$ is indeed generated by divisors dual to exceptional curves. □

3.5 Cox rings

Until now we introduced the total coordinate ring only in case of toric varieties in Remark 2.2.5. We also showed how to construct a toric variety as a quotient of the spectrum of its total coordinate ring in Theorem 2.2.4 and, for quotients of $\mathbb{C}^2$ by a cyclic group, in Proposition 3.3.8. Here we define the total coordinate ring in general and provide a geometric characterization, which will be used to describe this ring for surface quotient singularities. The content of this section is based on [ADHL10]. Let k be an algebraically closed field of characteristic 0.
As usual, a divisorial sheaf $\mathcal{O}_X(D)$ is defined by taking for an open subset $U \subset X$

$$\Gamma(U, \mathcal{O}_X(D)) = \{f \in k(X)^* \colon (div(f) + D)|_U \geq 0\} \cup \{0\}$$

with natural restrictions.

Definition 3.5.1. Let X be a normal variety with a free finitely generated class group. The **Cox ring** (or the **total coordinate ring**) of X is a $\mathrm{Cl}(X)$-graded module

$$\mathrm{Cox}(X) = \bigoplus_{[D] \in \mathrm{Cl}(X)} \Gamma(X, \mathcal{O}_X(D)),$$

where sections are multiplied as rational functions on X.

More precisely, we choose compatible representatives of divisor classes, that is we fix a subgroup K of the group of Weil divisors of X such that the canonical map $c \colon K \to \mathrm{Cl}(X)$ sending a divisor $D \in K$ to its class $[D] \in \mathrm{Cl}(X)$ is an isomorphism. Then $\mathcal{O}_X(D)$ is in fact understood as $\mathcal{O}_X(c^{-1}([D]))$. However, different choices of representatives of divisor classes give isomorphic ring structures – for the details see [ADHL10, Sect. 4.1].

Remark 3.5.2. If X is a normal variety with a finitely generated class group which is not free then the Cox ring of X can also be defined, see [ADHL10, Sect. 4.2]. The module structure is, as before, the sum of rings of sections of $\mathcal{O}_X(D)$ where D runs through a set of chosen representatives of classes of Weil divisors. However, to define multiplication, one has to look into the group structure more carefully, which we skip. In fact, the only case in which a non-free class group appears is the computation of the Cox ring of a quotient singularity in section 5.1, which is not essential for our exposition.

A few interesting properties of Cox rings can be proven directly from the definition. For example, the following theorem assures that a Cox ring of a variety cannot be arbitrarily bad.

Theorem 3.5.3. *[ADHL10, Thm 5.1.1] Let X be a normal variety with only constant invertible functions and finitely generated class group. Then its Cox ring is an integral and normal ring.*

However, a Cox ring of a variety does not have to be finitely generated. The question about the existence of a finite generating set of a Cox ring is very basic and one of the most important questions in this theory. The results are interesting already in dimension 2, see e.g. [AHL10] for the criterion in case of K3 surfaces. In the next chapter we give an answer to this question in case of surface quotient singularities by proving that their Cox rings are quotients of polynomial rings by principal ideals, see Theorem 4.3.3. Moreover, in chapter 5 we provide a method of describing a generating set of a Cox ring of a surface quotient singularity (see Theorem 5.2.9), which is likely to generalize to higher dimensions (at least for some classes of groups), where the construction of a resolution is often unknown and obtaining the result similar to Theorem 4.3.3 seems difficult.
In the proof of Theorem 4.3.3 we use the geometric characterization of the Cox ring, given below, preceded by a few definitions.

Definition 3.5.4. [ADHL10, Def. 2.1.1] A **quasitorus** is an affine algebraic group H whose algebra of regular functions $\Gamma(H, \mathcal{O}_H)$ is generated as a k-vector space by the characters of H. A **torus** is a connected quasitorus.

The standard torus $(k^*)^n$ is a torus in the sense of the definition above. This will be the only case considered throughout this text.

Definition 3.5.5. [ADHL10, Sect. 5.3] A variety Z with an action of a quasitorus H is **H-factorial** if every H-invariant Weil divisor on Z is principal.

Definition 3.5.6. [ADHL10, Def. 6.4.1] Let an affine algebraic group G act on a variety W. We say that this action is **strongly stable** if there is an open invariant subset $W' \subseteq W$ such that

1. the complement $W \setminus W'$ is of codimension at least two in W,
2. the group G acts freely (i.e. with trivial isotropy groups) on W',
3. for every $x \in W'$ the orbit $G \cdot x$ is closed in W.

Theorem 3.5.7. *[ADHL10, Cor. 6.4.4] Let Z be a normal affine variety with an action of a quasitorus H. Assume that*

1. *every invertible function on Z is constant,*
2. *Z is H-factorial,*
3. *there exists an open H-invariant subset $W \subseteq Z$ with $\operatorname{codim}_Z(Z \setminus W) \geq 2$ such that the action of H on W is strongly stable and admits a good quotient $q\colon W \to X$.*

Then Z is the total coordinate space of X, i.e. the spectrum of the Cox ring of X.

This result allows us to proceed as follows: first we find a finitely generated ring R, which is a candidate for the Cox ring of considered minimal resolution X of $\mathbb{C}^2/G$, and consider its spectrum $Z = \mathrm{Spec}(R)$. Then we define a (quasi)torus action on Z such that a (geometric) quotient W/H of some open subset $W \subset Z$ is isomorphic to X. After we have proved the properties of the action listed above, we know that $Z = \mathrm{Spec}(\mathrm{Cox}(X))$, i.e. $R = \mathrm{Cox}(X)$.

Chapter 4

The relation in the Cox ring

This chapter is devoted to the proof of Theorem 4.3.3 which describes the Cox ring of the minimal resolution X of a surface quotient singularity $\mathbb{C}^2/G$ as a quotient of a polynomial ring by a principal ideal. The main tool is the geometric characterization of the Cox ring, see Theorem 3.5.7.
We start from introducing a torus action on an affine space and defining an invariant hypersurface, which is the candidate S for the spectrum of the Cox ring. Then, in section 4.2 we deal with the most difficult part of the proof, i.e. that an open subset of S admits a good quotient onto X. The embedding of S in an affine space, equivariant with respect to the torus action defined in section 4.1, gives us an embedding of X in a 3-dimensional toric variety, as in e.g. [HK00, Prop. 2.11] and [ADHL10, Sect. III.2.5]. In section 4.3 we check the remaining conditions required by Theorem 3.5.7 to finish the proof that indeed $S \simeq \mathrm{Spec}(\mathrm{Cox}(X))$.

4.1 The Picard torus action

Let n be the number of components of the exceptional divisor of the minimal resolution X of $\mathbb{C}^2/G$ for a small subgroup $G < GL(2,\mathbb{C})$.

Definition 4.1.1. The torus

$$T = \mathrm{Hom}(\mathrm{Pic}(X), \mathbb{C}^*) = \mathrm{Hom}(\mathrm{Cl}(X), \mathbb{C}^*) \simeq (\mathbb{C}^*)^n$$

will be called the **Picard torus** of the minimal resolution X.

We define the action of the Picard torus T on $\mathbb{C}^{n+3}$ and investigate geometric quotients of open subsets of this affine space. In section 4.1.3 we propose a candidate for the $\mathrm{Spec}(\mathrm{Cox}(X))$, defined as a hypersurface in $\mathbb{C}^{n+3}$, and prove that it is invariant under the action of T in order to consider quotients of this action in section 4.2.
To define the action of T on $\mathbb{C}^{n+3}$ we use the extended intersection matrix U, described in Notation 3.4.5. We fix the coordinates: let

$$\mathbb{C}[y_0, y_{1,1}, \ldots, y_{1,n_1}, x_1, y_{2,1}, \ldots, y_{2,n_2}, x_2, y_{3,1}, \ldots, y_{3,n_3}, x_3]$$

be the coordinate ring of $\mathbb{C}^{n+3}$.

Definition 4.1.2. Define a Picard torus action $T \times \mathbb{C}^{n+3} \to \mathbb{C}^{n+3}$ by the formula

$$(\underline{t}, \underline{x}) = ((t_1, \dots, t_n), (y_0, y_{1,1}, \dots, y_{3,n_3}, x_3)) \mapsto$$
$$\mapsto (\underline{t}^{u_0} \cdot y_0, \underline{t}^{u_1} \cdot y_{1,1}, \dots, \underline{t}^{u_{n-1}} \cdot y_{3,n_3}, \underline{t}^{u_n} \cdot x_3)$$

where u_i is the i-th column of U and $\underline{t}^{u_i} = t_1^{(u_i)_1} \cdots t_n^{(u_i)_n}$.

Remark 4.1.3. In other words, this is the composition of a homomorphism of tori $T \to (\mathbb{C}^*)^{n+3} \subset \mathbb{C}^{n+3}$ defined by U^t with a natural action of $(\mathbb{C}^*)^{n+3}$ on $\mathbb{C}^{n+3}$, similarly as in Remark 3.3.9.

Before we move to considering certain quotients of open subsets of $\mathbb{C}^{n+3}$ by this action (see section 4.1.2), we need some technical results. In section 4.1.1 we determine the kernel of the lattice map given by U, which appears later, when we use the toric geometry setting.

4.1.1 The kernel map

We look at U as at the restriction of a map from $\mathbb{R}^{n+3}$ to $\mathbb{R}^n$ (in the standard basis) to the sublattice $\mathbb{Z}^{n+3} \subset \mathbb{R}^{n+3}$. By $\ker U$ we understand the sublattice of $\mathbb{Z}^{n+3}$ carried to 0 by U. The aim of this section is to describe a convenient set of its generators.

Definition 4.1.4. Let A be a square matrix. Then A' denotes A with a new column $(0, \dots, 0, 1)^t$ added on the right, A'' denotes A' with a new column $(1, 0, \dots, 0)^t$ added on the left:

$$A' = \left(\begin{array}{c|c} & 0 \\ A & \vdots \\ & 0 \\ & 1 \end{array}\right) \qquad A'' = \left(\begin{array}{c|c|c} 1 & & 0 \\ 0 & A & \vdots \\ \vdots & & 0 \\ 0 & & 1 \end{array}\right)$$

These operations will be applied to matrices A_i describing the branches of the exceptional divisor of X. We can think of A_i'' as if we cut out from U the block A_i with the suitable parts of the first column and the column just after A_i.
We will frequently use the following term:

Definition 4.1.5. Vector $\xi = (\xi_1, \dots, \xi_{n_i+1}) \in \mathbb{Z}^{n_i+1}$ is **orthogonal to the i-th branch**, of length n_i, represented by the matrix A_i, if $\xi_1 = 1$ and $A_i'\xi = 0$.

Lemma 4.1.6. *There exists a unique vector α_i orthogonal to the i-th branch of the exceptional divisor of the minimal resolution of a surface quotient singularity. It has integral and non-negative entries, which form an increasing sequence.*

Proof. The consecutive entries of $\alpha_i = (1, z_1, \dots, z_{n_i})$ can be computed from the form of A_i like that:

$$\begin{aligned} z_1 &= a_{i,1} \in \mathbb{Z}, \\ z_2 &= a_{i,2} z_1 - 1 \in \mathbb{Z}, \\ z_3 &= a_{i,3} z_2 - z_1 \in \mathbb{Z}, \dots \\ z_k &= a_{i,k} z_{k-1} - z_{k-2} \in \mathbb{Z}, \dots \end{aligned}$$

Hence by induction all entries of α_i are uniquely determined and integral. Moreover, $a_{i,j} > 1$ since they are entries of a Hirzebruch-Jung continued fraction, so $z_k \geq z_{k-1} + (z_{k-1} - z_{k-2})$ and again by induction the sequence (z_i) is increasing and all its elements are positive. □

Notation 4.1.7. In what follows α_i will always denote the unique vector orthogonal to the i-th branch of the exceptional divisor.

Now let us construct a basis of $\ker U$.

Notation 4.1.8. Elements of $\ker U$ will be presented as quadruples (u, w_1, w_2, w_3) consisting of a number u and three vectors w_i of lengths $n_i + 1$ respectively, i.e.

$$(u, w_1, w_2, w_3) := (u, (w_1)_1, \dots, (w_1)_{n_1+1}, (w_2)_1, \dots, (w_2)_{n_2+1}, (w_3)_1, \dots, (w_3)_{n_3+1}).$$

Such a partition is natural: when we multiply U by a vector of this form, the number u is multiplied by the numbers in the column corresponding to the branching point of the resolution diagram, and the remaining three parts correspond to the branches. Thus obviously

$$v_2 = (0, \alpha_1, 0, -\alpha_3) \quad \text{and} \quad v_3 = (0, 0, \alpha_2, -\alpha_3)$$

are in $\ker U$. We construct v_1 such that $\{v_1, v_2, v_3\}$ is a basis of $\ker U$.

Lemma 4.1.9. *There is a unique vector $v \in \ker U$ of the form*

$$(1, (0, *, \dots, *), (0, *, \dots, *), (d, *, \dots, *))$$

where $*$ stands for an integer and $-d$ is the self-intersection number of the central curve in the exceptional divisor of the minimal resolution.

Proof. First note that for any $a, b \in \mathbb{Z}$ there is a unique integral vector in the kernel of A''_i of the form $(a, b, *, \dots, *)$. To see this, we just determine the entries by an inductive procedure as in the proof of Lemma 4.1.6.
Consider vectors in kernels of A''_i of two types:

$$\beta_i = (1, 0, *, \dots, *) \qquad \text{and} \qquad \gamma_i = (1, d, *, \dots, *). \tag{4.1.1.1}$$

In addition, again as in the proof of Lemma 4.1.6, we see that the entries of each β_i form a decreasing sequence and the entries of each γ_i form an increasing sequence. By $\overline{\beta_i}$ and $\overline{\gamma_i}$ we denote vectors constructed from β_i and γ_i by removing the first entry. Look at

$$v = (1, \overline{\beta_1}, \overline{\beta_2}, \overline{\gamma_3}),$$

and compute $U \cdot v$. Since each $\overline{\beta_i}$ starts from 0 and $\overline{\gamma_i}$ from d, the first entry of $U \cdot v$ is 0. Following entries are the same as the entries of first $A''_1 \cdot \beta_1$, then $A''_2 \cdot \beta_2$ and finally $A''_3 \cdot \gamma_3$, so they are also 0.
Finally, v is uniquely determined, because if we write $v = (u, w_1, w_2, w_3)$ then from the form of U we see that $(u, (w_i)_1, \dots, (w_i)_{n_i+1})$ must be in the kernel of A''_i, so it is uniquely determined by u and $(w_i)_1$ for $i = 1, 2, 3$. □

Notation 4.1.10. Take $v_1 = v$ from the above lemma and write v_1, v_2, v_3 in the rows of a matrix K, divided into blocks in a similar way as U in Notation 4.1.8.

$$K = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \left(\begin{array}{c|c|c|c} 1 & 0,*,\ldots,* & 0,*,\ldots,* & d,*,\ldots,* \\ 0 & \alpha_1 & 0 & -\alpha_3 \\ 0 & 0 & \alpha_2 & -\alpha_3 \end{array}\right) = \left(\begin{array}{c|c|c|c} 1 & \overline{\beta_1} & \overline{\beta_2} & \overline{\gamma_3} \\ 0 & \alpha_1 & 0 & -\alpha_3 \\ 0 & 0 & \alpha_2 & -\alpha_3 \end{array}\right)$$

The choice of the matrix K defining the kernel of U is obviously non-unique; we choose one that is convenient for further computations.

Remark 4.1.11. Notice that K indeed defines the kernel of the lattice map, not only the map of vector spaces, i.e. v_1, v_2, v_3 span a full sublattice of $\mathbb{Z}^{n+3}$. This is because K has an identity matrix as a minor, since α_1 and α_2 start from 1 by Lemma 4.1.6.

4.1.2 The toric structure of quotients by the action of T

We investigate geometric quotients of open subsets of $\mathbb{C}^{n+3}$ by the action of the Picard torus T using toric geometry as a tool. More precisely, what we do is the reverse of the toric quotient construction (Theorem 2.2.4). Instead of expressing a given toric variety as a quotient of an open set of an affine space, we reconstruct this variety and the open set knowing the torus action on an affine space. Obviously, it is not unique, hence we recover only some properties and then it turns out that remaining parameters can be chosen arbitrarily.
We think of the Picard torus T as of a subtorus of the big torus $(\mathbb{C}^*)^{n+3} \subset \mathbb{C}^{n+3}$ – the embedding is given by U^t (see Remark 4.1.3; this is an embedding since columns of U generate $\mathbb{Z}^n$). Look at the short exact sequence of the torus embedding

$$0 \longrightarrow T \longrightarrow (\mathbb{C}^*)^{n+3} \longrightarrow (\mathbb{C}^*)^3 \longrightarrow 0.$$

Let

$$M' \simeq \mathbb{Z}^{n+3} \quad \text{and} \quad M \simeq \mathbb{Z}^3$$

be the lattices of characters of the big torus $(\mathbb{C}^*)^{n+3} \subset \mathbb{C}^{n+3}$ (with the same fixed coordinates) and of the quotient torus respectively. By P we denote the monomial lattice of T, which can be identified with the Picard group of X. Then we have a map of monomial lattices

$$0 \longrightarrow M \longrightarrow M' \xrightarrow{U} P \longrightarrow 0, \tag{4.1.2.1}$$

where M can be identified with $\ker U \subset M'$ and we may assume that the map $M \to M'$ is given in standard coordinates by K^t, where K is as in Notation 4.1.10. Thus we have described the monomial lattice M of a quotient variety. To understand more of its structure we prefer to look at the dual exact sequence

$$0 \longrightarrow P^\vee \xrightarrow{U^t} N' \xrightarrow{K} N \longrightarrow 0$$

(note that it is exact on both ends, because M is a saturated sublattice of M', i.e. the quotient is torsion free). We first describe the set of rays of the fan of a quotient and then look which points have to be removed from $\mathbb{C}^{n+3}$ to obtain a chosen variety with good properties as a geometric quotient. (In other words, we will check which points of $\mathbb{C}^{n+3}$ are unstable with respect to chosen linearizations of the action.)

Notation 4.1.12. When we choose one of many possible geometric quotients of $\mathbb{C}^{n+3}$ by T, a fan of such a quotient will be denoted by Σ. And by Σ' we will denote the fan of $\mathbb{C}^{n+3}$ in N': the positive orthant and all its faces.

We sum up the discussion above in the following observation.

Corollary 4.1.13. *Look at the third arrow in the sequence above:* $N' \xrightarrow{K} N$. *The rays of* Σ *are the images of the rays of* Σ' *under the map given by* K*, so their coordinates are just columns of* K.

Some more information on the structure of fans of quotients can be obtained based on this observation. Let x, y, z be the coordinates in $N_{\mathbb{R}} = N \otimes \mathbb{R}$ corresponding to the standard basis in N.

Lemma 4.1.14. *A fan* $\Sigma \subset N_{\mathbb{R}}$ *with the set of rays as in Corollary 4.1.13 has the following properties:*

1. *the rays of* Σ *are divided into three groups, corresponding to the branches of the diagram, of vectors lying in three planes:* $y = 0$, $z = 0$ *and* $y = z$,
2. *the intersection of these planes is the line* $y = z = 0$*, represented in* $\Sigma(1)$ *by the central ray* $(1, 0, 0)$*, the first column of* K,
3. *the rays in each group together with* $(1, 0, 0)$*, when considered as vectors not in* $N_{\mathbb{R}}$*, but in the plane containing them, form the 1-skeleton of a fan of the minimal resolution of a cyclic quotient singularity. In particular, adjacent rays in each group span the intersection of* N *with the plane containing this group.*

Proof. Statements 1. and 2. follow directly from the definition of K (see Notation 4.1.10).
To prove the last one we construct matrices K_i for $i = 1, 2, 3$ by taking from K the first column and the i-th of remaining blocks from division in Notation 4.1.10. Then columns of K_i are rays of the i-th group. The isomorphism of the plane containing the i-th group of rays with $\mathbb{Z}^2$ can be defined e.g. by forgetting about the last coordinate for $i = 1, 3$ and forgetting about the second one for $i = 2$. This corresponds to constructing matrices $\overline{K_i}$ from K_i by forgetting the last row for $i = 1, 3$ and the second one for $i = 2$:

$$K_1 = \begin{pmatrix} 1 & \overline{\beta_1} \\ 0 & \alpha_1 \end{pmatrix} \qquad K_2 = \begin{pmatrix} 1 & \overline{\beta_2} \\ 0 & \alpha_2 \end{pmatrix} \qquad K_3 = \begin{pmatrix} 1 & \overline{\gamma_3} \\ 0 & -\alpha_3 \end{pmatrix}.$$

By construction of α_i, β_i, γ_i rows of K_i span the lattice kernel of the map given by A''_i. Hence, by Proposition 3.3.8, columns of K_i are rays of the fan of the minimal resolution of the cyclic quotient singularity corresponding to A_i (i.e. to the continued fraction with entries on the diagonal of A_i). □

Definition 4.1.15. By the **outer rays** of Σ we understand the set consisting of three rays which are the last columns of K in each block consisting of more then one rays. Sometimes we use the name **inner rays** for the remaining ones. The first column $(1, 0, 0)$ will be called the **central ray**.

Notation 4.1.16. In what follows we will say that a ray lies on the i-th branch if it is a column from the i-th block of K (excluding the one consisting only of the central ray). We assume that the central ray belongs to all three branches.

In the following lemma we describe the outer rays of Σ in terms of Hirzebruch-Jung continued fractions assigned to branches of the resolution diagram in Definition 3.4.2.

Lemma 4.1.17. *Assume that the self-intersection numbers of the components of the i-th branch of the exceptional divisor are the negatives of the entries of a Hirzebruch-Jung continued fraction p_i/q_i, and that $-d$ is the self intersection number of the central curve. Then the outer rays are*

$$(dp_3 - q_3, -p_3, -p_3), \quad (-q_2, 0, p_2), \quad (-q_1, p_1, 0).$$

Proof. We have to find formulae for the last entries of vectors α_i, β_i, γ_i introduced in the proofs of Lemmata 4.1.6 and 4.1.9.
First of all we notice that the recursive formula for the entries of α_i, given in the proof of Lemma 4.1.6, is also a formula for the numerator of the reversed continued fraction. More precisely, if $p_i/q_i = [a_{i,1}, \ldots, a_{i,n_i}]$, and α_i is orthogonal to the i-th branch, then $(\alpha_i)_{j+1}$ is the numerator of $[a_{i,n_i}, a_{i,n_i-1}, \ldots, a_{i,n_i-j+1}]$ for $j \in \{1, \ldots, n_i\}$. But the reversed continued fraction to p_i/q_i is p_i/q_i' where q_i' is reverse modulo p to q_i – this and other useful facts on Hirzebruch-Jung continued fractions can be found in [CLS11, Section 10.2]. Thus $(\alpha_i)_{n_i+1} = p_i$.
The case of β_i from formula (4.1.1.1) is very similar. If we write down an analogous formula for its entries, we obtain that the last one is the negative of the numerator of $[a_{i,n_i}, \ldots, a_{i,2}]$, which is the same as the negative of the numerator of $[a_{i,2}, \ldots, a_{i,n_i}] = r_i/s_i$. But

$$\frac{p_i}{q_i} = a_{i,1} - \frac{1}{\frac{r_i}{s_i}},$$

so indeed $r_i = q_i$ and β_i ends with $-q_i$.
Let $\alpha_i' = (0, (\alpha_i)_1, \ldots, (\alpha_i)_{n_i+1})$. Then $\gamma_i = \beta_i + d\alpha_i'$, because each of these vectors is uniquely determined by their first two entries (as shown in the proof of Lemma 4.1.9), and these entries satisfy this equality. Therefore γ_i ends with $dp_i - q_i$. □

Remark 4.1.18. Let $G = BD_{n,m}$. Then using [Bri68, Satz 2.11] one can see that the last entry of γ_i can be written as $m + p_3$, so the first outer ray is $(m + p_3, -p_3, -p_3)$.

Lemma 4.1.19. *The outer rays span a convex cone which contains* $(1, 0, 0)$ *inside.*

Proof. We show that $(1, 0, 0)$ is a positive combination of the outer rays. We have

$$\frac{p_3}{p_1}(-q_1, p_1, 0) + \frac{p_3}{p_2}(-q_2, 0, p_2) + (dp_3 - q_3, -p_3, -p_3) = p_3(d - \frac{q_3}{p_3} - \frac{q_1}{p_1} - \frac{q_2}{p_2})(1, 0, 0),$$

so it suffices to prove that

$$d - \frac{q_1}{p_1} - \frac{q_2}{p_2} - \frac{q_3}{p_3} > 0.$$

If $d \geq 3$ this is obvious, because $q_i < p_i$. And if $d = 2$, this can be checked case by case using the table in [Bri68, Satz 2.11], in which the continued fraction are assigned to group structures. The cases where this number is smallest are the quotient by the subgroups of $SL(2, \mathbb{C})$. □

Notation 4.1.20. We want to consider only fans $\Sigma \subset N_{\mathbb{R}}$ with the set of rays as described in Corollary 4.1.13 and such that the (set-theoretical) sum of all cones in Σ (the support of Σ) is the convex cone spanned by the outer rays. Also, we consider only simplicial fans. From now on Σ will denote a fan satisfying these conditions.

The choice of such a fan corresponds to the choice of the quotient X_Σ of an open subset of $\mathbb{C}^{n+3}$ by T. More precisely, X_Σ is a geometric quotient of $\mathbb{C}^{n+3} \setminus Z(\Sigma)$ by T, where $Z(\Sigma)$ is the zero set of the irrelevant ideal of Σ. Since only simplicial fans are admitted, these quotients are geometric. The structure of $Z(\Sigma)$ is studied in more detail in section 4.2.1.
It turns out that some 2- and 3-dimensional cones have to belong to a fan Σ satisfying the conditions of Notation 4.1.20, independently of the choice.

Lemma 4.1.21. Σ *contains the following cones:*

1. *all faces spanned by two adjacent rays in one of the planes* $y = 0$, $z = 0$, $y = z$,
2. *faces* $\sigma((0,1,0),(0,0,1))$, $\sigma((0,1,0),(d,-1,-1))$, $\sigma((0,0,1),(d,-1,-1))$,
3. *3-dimensional cones containing the central ray:* $\sigma((1,0,0,),(0,1,0),(0,0,1))$, $\sigma((1,0,0),(0,0,1),(d,-1,-1))$, $\sigma((1,0,0),(0,1,0),(d,-1,-1))$.

Moreover, the cones containing the central ray are smooth and the divisor associated with the central ray is a $\mathbb{P}^2$.

Proof. See Fig. 4.1 for a picture of a plane section of the cone spanned by the outer rays and the cones mentioned in the lemma.
First assume that the cone spanned by two adjacent rays ρ and ρ' from one branch is not in Σ. Let ρ be nearer to the central ray $(1,0,0)$. Then there exists a cone in Σ spanned by ρ, ρ_1, ρ_2 such that each of these rays comes from a different branch – otherwise ρ would not be in the interior of the support of Σ. But $\sigma(\rho, \rho_1, \rho_2)$ contains $(1,0,0)$ in the interior, because $(1,0,0)$ is inside the cone spanned by the outer rays and all the rays lie on three planes intersecting in the central ray, hence we get a contradiction.
As for the cones listed in (2) and (3), they must be in Σ, since the rays $(0,1,0)$, $(0,0,1)$ and $(d,-1,-1)$ are the only three which can span a cone with $(1,0,0)$, which lies in the interior of the cone spanned by the outer rays.
If we choose any pair of vectors from $(0,1,0)$, $(0,0,1)$, $(d,-1,-1)$ and take $(1,0,0)$ as the third one, obviously we get a triple that generates the whole lattice, so the central part of our picture consists indeed of three smooth cones.

To describe the structure of the divisor associated with the central ray $(1, 0, 0)$ of this fan one has to project cones containing it to the orthogonal plane $x = 0$ (see [CLS11, Proposition 3.2.7]). The result is the fan which has $(1, 0)$, $(0, 1)$ and $(-1, -1)$ as rays and contains all three possible 2-dimensional cones, hence the fan of a smooth $\mathbb{P}^2$. □

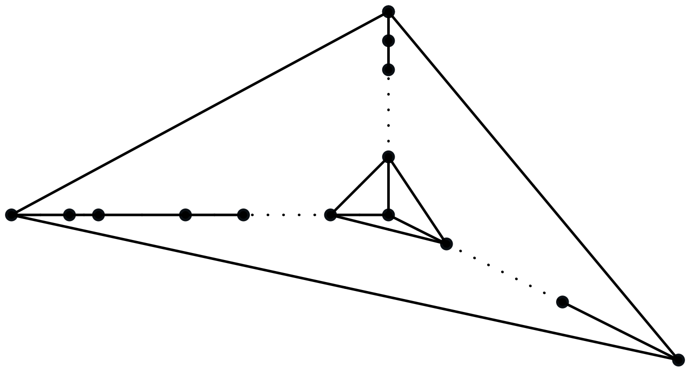


Figure 4.1: Faces that have to be in Σ (shown in a section)

Fig. 4.1 is a schematic picture of a section of the cone spanned by the outer rays with the sections of faces mentioned in Lemma 4.1.21 included. All considered fans Σ correspond to triangulations of this diagram. Toric varieties obtained this way are different geometric quotients of open subsets of $\mathbb{C}^{n+3}$ by T. In general there is no smooth model, for example because of the fact that the cones containing the faces of the cone spanned by the outer rays are most often non-smooth.

4.1.3 The candidate for Spec(Cox(X))

We introduce a hypersurface $S \subset \mathbb{C}^{n+3}$, which is our candidate for the spectrum of the Cox ring of the minimal resolution of $\mathbb{C}^2/G$. Its equation can be determined from the resolution diagram together with the self-intersection numbers of the components of the special fibre. We prove that it is invariant under the Picard torus action.

Construction 4.1.22. We define a hypersurface $S \subset \mathbb{C}^{n+3}$ by describing its ideal

$$I(S) \subset \mathbb{C}[y_0, y_{1,1}, \ldots, y_{1,n_1}, x_1, y_{2,1}, \ldots, y_{2,n_2}, x_2, y_{3,1}, \ldots, y_{3,n_3}, x_3],$$

which is generated by a single trinomial equation. Each monomial of this equation corresponds to one branch of the resolution diagram. The variables, except y_0, are divided into three sequences

$$(y_{i,1}, y_{i,2}, \ldots, y_{i,n_i-1}, y_{i,n_i}, x_i)$$

for $i = 1, 2, 3$, and all variables in the i-th sequence appears only in the monomial corresponding to the i-th branch. As the i-th vector of exponents we take the vector α_i orthogonal to the i-th branch, so the equation is

$$\sum_{i=1,2,3} y_{i,1}^{(\alpha_i)_1} \cdots y_{i,n_i}^{(\alpha_i)_{n_i}} \cdot x_i^{(\alpha_i)_{n_i+1}} = 0. \tag{4.1.3.1}$$

It can be easily seen that the hypersurface defined by this equation is irreducible.

Remark 4.1.23. In Lemma 4.1.6 we proved that all entries of each α_i are positive integers and that $(\alpha_i)_1 = 1$. Hence the equation above is indeed a polynomial and variables $y_{1,1}, y_{2,1}, y_{3,1}$ appear with exponent 1.

The choice of coefficients of monomials equal to 1 is arbitrary. For any other set of coefficients we would just obtain a different embedding of $\mathrm{Spec}(\mathrm{Cox}(X))$ in $\mathbb{C}^{n+3}$.

Example 4.1.24. In the case of Du Val singularities the equation is formed as follows: for each variable its exponent is equal to the distance of the corresponding vertex in the resolution diagram from the branching point (we may assume that x_i corresponds to a leaf added at the end of the i-th branch, so its distance from the branching point is the distance of y_{i,n_i} plus 1). For example, let us look at E_8 singularity $\mathbb{C}^2/BI$. The extended intersection matrix is

$$U(BI) = \left(\begin{array}{c|cc|ccc|ccccc}
-2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \hline
1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline
1 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline
1 & 0 & 0 & 0 & 0 & 0 & -2 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1
\end{array}\right)$$

and the kernel matrix with the rays of $\Sigma(BI)$ as columns is

$$K(BI) = \left(\begin{array}{c|cc|ccc|ccccc}
1 & 0 & -1 & 0 & -1 & -2 & 2 & 3 & 4 & 5 & 6 \\
0 & 1 & 2 & 0 & 0 & 0 & -1 & -2 & -3 & -4 & -5 \\
0 & 0 & 0 & 1 & 2 & 3 & -1 & -2 & -3 & -4 & -5
\end{array}\right)$$

The entries of vectors α_i, which are the exponents in the equation, can be read out from the second and third row of $K(BI)$:

$$S(BI) = \{y_{1,1}x_1^2 + y_{2,1}y_{2,2}^2x_2^3 + y_{3,1}y_{3,2}^2y_{3,3}^3y_{3,4}^4x_3^5 = 0\}$$

Example 4.1.25. Let us look at a group which is not in $SL(2,\mathbb{C})$: take $BD_{23,39}$, which appeared already in Example 3.4.4. We have

$$U(BD_{23,39}) = \left(\begin{array}{c|cc|cc|ccccc}
-3 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ \hline
1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline
1 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ \hline
1 & 0 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -3 & 1
\end{array}\right)$$

$$K(BD_{23,39}) = \left(\begin{array}{c|cc|cc|ccccc} 1 & 0 & -1 & 0 & -1 & 3 & 11 & 19 & 27 & 62 \\ 0 & 1 & 2 & 0 & 0 & -1 & -4 & -7 & -10 & -23 \\ 0 & 0 & 0 & 1 & 2 & -1 & -4 & -7 & -10 & -23 \end{array}\right)$$

and again we read out vectors α_i from $K(BD_{23,39})$ obtaining

$$S(BD_{23,39}) = \{y_{1,1}x_1^2 + y_{2,1}x_2^2 + y_{3,1}y_{3,2}^4 y_{3,3}^7 y_{3,4}^{10} x_3^{23} = 0\}.$$

Lemma 4.1.26. *The hypersurface S is invariant under the action of the Picard torus T from Definition 4.1.2.*

Proof. We look at the action of T on each monomial in the equation of S. The weights of this action are given by the columns of U, so to compute the weight vector of the action on the monomial corresponding to the i-th branch one multiplies U by $(0, \alpha_1, 0, 0)$, $(0, 0, \alpha_2, 0)$ and $(0, 0, 0, \alpha_3)$ respectively. Because α_i is orthogonal to the i-th branch, the result is $(1, 0, 0, \dots, 0)$, which means that T acts on each monomial, and therefore on the whole equation, by multiplication by t_0. Thus the set of zeroes of this equation is invariant under the action of T. □

Therefore we may consider geometric quotients of open subsets of S by T. They will be presented as subsets in different geometric quotients of open sets in $\mathbb{C}^{n+3}$ by T.

4.2 The resolution as a divisor in a toric variety

The aim of this section is to describe properties of certain geometric quotients of open subsets of hypersurface $S \subset \mathbb{C}^{n+3}$, introduced in Construction 4.1.22, by the Picard torus action. Let us fix a simplicial fan $\Sigma \subset \mathbb{R}^3$ satisfying conditions in Notation 4.1.20. In particular, its rays are columns of matrix K (see Notation 4.1.10). We consider an open subset of S obtained by removing zeroes of the irrelevant ideal (see Definition 2.2.3)

$$W = S \setminus Z(\Sigma) \subset \mathbb{C}^{n+3} \setminus Z(\Sigma)$$

and its quotient by the action of T.

Remark 4.2.1. As the quotient X_Σ of $\mathbb{C}^{n+3} \setminus Z(\Sigma)$ by T is geometric and $W = S \setminus Z(\Sigma)$ is a T-invariant closed subset of $\mathbb{C}^{n+3} \setminus Z(\Sigma)$, the quotient of W by T is also geometric (for example by [ADHL10, Proposition 2.3.9]).

Notation 4.2.2. We investigate the quotient $Y = W/T$ by looking at the embeddings which are horizontal arrows in the following diagram.

$$\begin{array}{ccc} W = S \setminus Z(\Sigma) & \hookrightarrow & \mathbb{C}^{n+3} \setminus Z(\Sigma) \\ \big\downarrow /T & & \big\downarrow /T \\ Y = W/T & \hookrightarrow & X_\Sigma \end{array}$$

We use toric geometry as a tool, because the right vertical arrow is a toric map. The first thing we prove is the smoothness of Y (see Proposition 4.2.6), which, roughly speaking, follows from the fact that the action of T on W is free and the smoothness of W. In section 4.2.2 we construct a birational morphism from Y to the quotient singularity $\mathbb{C}^2/G$. It comes from the embedding in a toric variety. Its existence implies that Y is a resolution of $\mathbb{C}^2/G$. However, at this point we do not know if it is the minimal resolution. This is proven in section 4.2.3 by computing intersection numbers of the irreducible components of the exceptional divisor of the constructed morphism to $\mathbb{C}^2/G$.

4.2.1 Smoothness of the quotient

The aim of this section is to prove Proposition 4.2.6, which states that the quotient $Y = W/T$ is smooth. In order to give the proof we first need to analyze the structure of the set $Z(\Sigma)$ of zeroes of the irrelevant ideal associated with the chosen fan Σ. Let us recall that the coordinates of $\mathbb{C}^{n+3}$ are denoted

$$y_0, y_{1,1}, \dots, y_{1,n_1}, x_1, y_{2,1}, \dots, y_{2,n_2}, x_2, y_{3,1}, \dots, y_{3,n_3}, x_3.$$

We say that y_0 corresponds to the central ray of Σ (i.e. is a monomial dual to the ray in a fan Σ' of $\mathbb{C}^{n+3}$ which maps to the central ray in Σ), $y_{i,j}$ corresponds to the j-th ray on the i-th branch and x_i corresponds to the i-th outer ray.

Lemma 4.2.3. *The set $W = S \setminus Z(\Sigma) \subset \mathbb{C}^{n+3}$ consists of three sets of points:*

1. *all points in S with all coordinates nonzero,*
2. *all points in S with one coordinate equal to zero,*
3. *all points in S with two coordinates equal to zero, such that these coordinates correspond to a pair of adjacent rays on one branch.*

It follows that W is independent of the choice of Σ.

Proof. The argument is a straightforward analysis of the structure of the irrelevant ideal $B(\Sigma) = \langle x^{\hat{\sigma}} : \sigma \in \Sigma_{max} \rangle$. Recall that $x^{\hat{\sigma}}$ is the product of variables corresponding to all the rays in $\Sigma(1)$ that are not in $\sigma(1)$. In our case Σ_{max} is the set of all 3-dimensional cones of Σ. Let us look at the number of coordinates equal to zero in a point in $Z(\Sigma)$.
First of all, if a point has ≥ 4 zeroes on different coordinates, or 2 or 3 zeroes on coordinates corresponding to the rays which do not span a cone in Σ, then for any cone $\sigma \in \Sigma_{max}$ one of these rays is not in σ, so $x^{\hat{\sigma}}$ evaluated at this point is 0. Hence all such points belong to $Z(\Sigma)$.
If a point $p \in S$ has 3 zeroes on coordinates corresponding to the rays whose images span a cone in Σ, then these rays lie on two different branches – i-th and j-th. But then monomials in the equation of S (see formula 4.1.3.1) which correspond to the i-th and j-th branch are 0 at p, so the third monomial also is 0 at p. Hence at least

one more coordinate of p is equal to zero. Thus $p \in Z(\Sigma)$, which implies that W does not contain any point with ≥ 3 zeroes.
The same argument works in the case where p has 2 zeroes on the coordinates corresponding to the rays from two different branches. Thus p with 2 zeroes can belong to W only if these zeroes are on the coordinates corresponding to adjacent rays from one branch.
We see that all such points p indeed belong to W: if we take $\sigma \in \Sigma_{max}$ containing all rays corresponding to zero coordinates of p, which is possible by Lemma 4.1.21, then $x^{\hat{\sigma}}(p) \neq 0$.
Therefore the only property of Σ on which W depends is the set of 2-dimensional cones spanned by adjacent rays on one branch. But Lemma 4.1.21 assures that this set is the same in all fans we consider, hence for any choice of Σ satisfying conditions of Notation 4.1.20 one obtains the same W. □

We need a following technical observation to prove that the action of T on W is free in Lemma 4.2.5.

Lemma 4.2.4. *Remove from the extended intersection matrix U any two columns corresponding to a pair of adjacent vertices on one branch of the resolution diagram. Then the remaining ones generate $\mathbb{Z}^n$.*

Proof. Let us denote by B_i for $i = 1, 2, 3$ the set of columns of U corresponding to the vertices on the i-th branch of the resolution diagram (hence the first column does not belong to any of these sets). Thus $|B_i| = n_i + 1$. By $e_0, \ldots, e_{n-1}$ we denote the standard basis of $\mathbb{Z}^n$.
The first case is when we remove two adjacent columns from one set. Without loss of generality we may assume that they lie in B_3. We perform reductions with integral coefficients on columns from the first set, in the same way as we computed entries of α_i in the proof of Lemma 4.1.6, but starting from the last column. This way we obtain that vectors $e_0, e_2, \ldots, e_{n_1}$ are in the lattice generated by the columns of U which were not removed. Similarly, by reducing B_2 we get e_0 and $e_{n_1+1}, \ldots, e_{n_1+n_2}$. Then look at the first column: it is $e_0 + e_1 + e_{n_1+1} + e_{n_1+n_2+1}$, so subtracting $e_0 + e_1 + e_{n_1+1}$ we get also $e_{n_1+n_2+1}$. Now there are two possibilities. If we removed the last column from B_3, we perform the same reductions in B_3 starting from $e_{n_1+n_2+1}$. If not, we reduce both starting from the first column and from the last one. In both cases it is easily seen that we obtain all the remaining vectors of the standard basis of $\mathbb{Z}^n$.
The second case, which is removing the first column of U and the first column in one set (let us take B_1), is even easier. As before, by linear combinations with integral coefficients, from B_2 and B_3 we obtain all corresponding standard basis vectors: $e_{n_1+1}, \ldots, e_{n-1}$, and also e_0. Thus we can perform reductions on B_1 starting from the last column and finish them using e_0 to obtain $e_1, \ldots, e_{n_1}$. □

Recall that the action of T on $\mathbb{C}^{n+3}$ is defined by the sequence of characters

$$\chi_i(\underline{t}) = \underline{t}^{u_i} = t_0^{(u_i)_0} \cdots t_{n-1}^{(u_i)_{n-1}}$$

for $i = 0, \ldots, n-1$, where u_i is the i-th column of U and $\underline{t} = (t_0, \ldots, t_{n-1}) \in T$.

Lemma 4.2.5. *T acts freely on W.*

Proof. We have to check that a point $p \in W$ cannot have nontrivial isotropy group. Assume that $\underline{t} = (t_0, \ldots, t_{n-1}) \in T$ is such that $\underline{t}p = p$. This means that all characters defining the action, except these corresponding to the coordinates equal to zero in p, give 1 evaluated at $\underline{t}$.
Our aim is to deduce that $t_i = 1$ for $i = 0, \ldots, n$ from the fact that $\chi_i(\underline{t}) = 1$ for indices i such that the i-th coordinate of p is nonzero. In other words, we would like to check when it is possible to obtain equalities $t_i = 0$ by multiplying equalities $\underline{t}^{u_i} = 1$ for i corresponding to nonzero coordinates of p. These operations are equivalent to operations on vectors of exponents in the lattice $\mathbb{Z}^n$. This can be reformulated as follows: if we remove from U the columns corresponding to the zero coordinates in p then the remaining columns span the lattice $\mathbb{Z}^n$. And, because p is of one of three types listed in Lemma 4.2.3, this result follows directly from Lemma 4.2.4. □

Proposition 4.2.6. *The quotient $Y = W/T$ is smooth.*

Proof. We prove that W is smooth by checking that all the singular points of S are in $Z(\Sigma)$. Indeed, if the Jacobian of the equation of S is zero in a point $(y_0, y_{1,1}, \ldots, x_1, y_{2,1}, \ldots, x_2, y_{3,1}, \ldots, x_3)$ then for each $i = 1, 2, 3$ at least one of the coordinates corresponding to a ray from the i-th branch is zero. Hence there are at least three coordinates equal to zero and, by Lemma 4.2.3, such a point is not in W. Since Y is a geometric quotient of a smooth variety by a free action of T, it is also smooth. A standard reference for such a statement is Luna's slice theorem, but we believe that this particular case can be much simpler. By the classical result of Sumihiro [Sum74] any point $w \in W$ has a T-invariant affine neighborhood and by applying Luna's theorem [Lun73] to this neighborhood we know that the quotient is smooth in the image of w. □

The smoothness of W/T can also be proven using the toric setting: the embedding of W/T in X_Σ, given by an equation in the Cox ring of X_Σ, and the toric localization (see Proposition 2.2.7). Below we sketch an alternate proof of Proposition 4.2.6 based on this idea. This proof reveals a special feature of quasi-reflections, important for understanding quotient singularities constructed via finite group action.

Proof. (Alternate proof of Proposition 4.2.6.) We investigate the smoothness locally, on the pieces of an affine cover of W/T corresponding to the set of maximal cones of Σ. Take any 3-dimensional cone $\sigma \in \Sigma$. By Lemma 4.1.21 its rays correspond to two adjacent points on one branch of the resolution diagram and one point on another branch. Thus, by Proposition 2.2.7, the localized equation is of the form

$$F(z_1, z_2, z_3) = z_1^{m_1} z_2^{m_2} + z_3^{m_3} + 1,$$

where z_1 and z_2 stand for either $y_{i,j}$ and $y_{i,j+1}$ or y_{i,n_i} and x_i, and $m_1, m_2, m_3 > 0$. The Jacobian matrix is

$$J(z_1, z_2, z_3) = (m_1 z_1^{m_1-1} z_2^{m_2}, m_2 z_1^{m_1} z_2^{m_2-1}, m_3 z_3^{m_3-1}).$$

If σ is a smooth cone then obviously there are no points for which both $F(z_1, z_2, z_3)$ and $J(z_1, z_2, z_3)$ are zero.
For the non-smooth cones the situation is a bit more complicated. Then U_σ is a quotient of $\mathbb{C}^3$ by an action of a (nontrivial) finite group H. The localized equation $F(z_1, z_2, z_3)$ gives a (ramified) covering $\overline{Z} = \{F = 0\}$ of an affine piece $Z = U_\sigma \cap (W/T)$, i.e. Z is a quotient of $\overline{Z}$ by H. We show that this action either has no points with nontrivial isotropy group or, if such points exists, the isotropy group acts on the tangent space by complex reflections, which means that the quotient is nonsingular by the Chevalley-Shephard-Todd theorem.
Applying a lattice automorphism if necessary, we may assume that two rays of σ correspond to two consecutive points from the second branch of the diagram and the last one to a point from the third branch:

$$\rho_1 = (a, 0, b), \quad \rho_2 = (c, 0, d), \quad \rho_3 = (e, f, f).$$

The map $\mathbb{Z}^3 \to N$ given in the standard basis by

$$e_1 \mapsto \overline{e_1} = (a, 0, b), \quad e_2 \mapsto \overline{e_2} = (c, 0, d), \quad e_3 \mapsto \overline{e_3} = (e, f, f)$$

defines the toric morphism $\mathbb{C}^3 \to U_\sigma$, a quotient by H, which is the cokernel: $\mathbb{Z}^3 \to N \to H \to 0$. It can be checked easily that H is cyclic, generated by the class of $(0, 1, 0) \in N$.
The computations done in the case of a smooth cone show that $\overline{Z}$ is nonsingular. Assume that there are points in $\overline{Z}$ with nontrivial isotropy group. We need to find the weights of the action of H on the coordinates z_1, z_2, z_3 in $\mathbb{C}^3$ corresponding to ρ_1, ρ_2, ρ_3. The class of $(0, 1, 0) \in N$ generates H, so the weight of the action on z_i is $(0, 1, 0) \cdot \overline{e_i}^\vee$. We have

$$\overline{e_1}^\vee = (d, c - \frac{-ed}{f}, -c), \quad \overline{e_2}^\vee = (-b, \frac{eb}{f} - a, a), \quad \overline{e_3}^\vee = (0, \frac{1}{f}, 0).$$

Thus a generator of H acts on z_1, z_2, z_3 by $\operatorname{diag}(\xi^{-ed}, \xi^{eb}, \xi)$, where ξ is a primitive f-th root of unity, so if (z_1, z_2, z_3) has a nontrivial isotropy group, then $z_3 = 0$. Hence a generator of the isotropy group acts by $\operatorname{diag}(1, 1, \xi^r)$ for some $r \in \mathbb{Z}$.
At a point with a nontrivial isotropy group, hence of the form $(z_1, z_2, 0)$, the tangent space is spanned by $(0, 0, 1)$ and some vector of the form $(p, q, 0)$, where $p, q \neq 0$. Since both are the eigenvectors of the action of H and only the second one corresponds to eigenvalue 1, the isotropy group indeed acts by complex reflections. □

4.2.2 The quotient is a resolution of $\mathbb{C}^2/G$

An embedding of the geometric quotient $Y = W/T$ in a toric variety X_Σ (see the diagram in Notation 4.2.2) leads to a construction of a birational morphism $Y \to \mathbb{C}^2/G$, shown below. We start from describing the toric morphism of ambient spaces.

Let $\Delta \subset N_{\mathbb{R}}$ denote the fan consisting of a cone spanned by the outer rays of Σ and all its faces. As before, $\Sigma' \subset N'_{\mathbb{R}}$ is the standard fan of $\mathbb{C}^{n+3}$. Look at the composition π of two fan morphisms: $\Sigma' \to \Sigma$, given by the matrix K (as in Notation 4.1.10) and $\Sigma \to \Delta$, induced by the identity on N. This last homomorphism – forgetting about all rays except the outer ones – is a proper birational morphism of X_{Σ} to an affine variety, which contracts torus invariant divisors corresponding to the omitted rays.

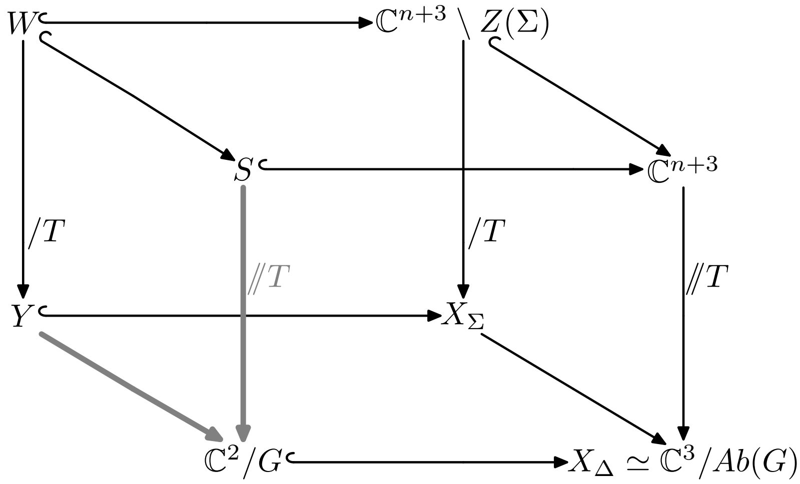
Lemma 4.2.7. *The toric morphism $\mathbb{C}^{n+3} \to X_{\Delta}$ induced by π is a good categorical quotient (as in Definition 2.2.1) by the Picard torus action and $\mathbb{C}^{n+3}/\!/T = X_{\Delta} \simeq \mathbb{C}^3/Ab(G)$.*

Proof. Recall the exact sequence of lattices 4.1.2.1 describing the Picard torus action on $\mathbb{C}^{n+3}$ – it is the upper horizontal exact sequence in the diagram below. The invariant monomials of this action are lattice points in the intersection of M with the positive orthant in M'. Hence, looking at dual lattices, the good categorical quotient $\mathbb{C}^{n+3}/T$ is the affine toric variety corresponding to the image of the positive orthant in $\pi\colon N' \to N$, that is X_{Δ} (see e.g. [CLS11, Prop. 5.0.9]). We will now prove that X_{Δ} is isomorphic to $\mathbb{C}^3/Ab(G)$.
The left vertical sequence is just dividing the monomial lattice M' of $\mathbb{C}^{n+3}$ by a sublattice spanned by these basis elements which correspond to inner rays. That is, $M'' \simeq \mathbb{Z}^3$ and we consider the positive octant in this lattice, which is the image of Σ'. In the right one the quotient of $\mathrm{Pic}(X)$ by the subgroup of divisors contracted by the resolution of the singularity is just $\mathrm{Cl}(\mathbb{C}^2/G)$, which is $Ab(G)$ by Proposition 3.4.8.

$$
\begin{array}{ccccccccc}
 & & & & 0 & & 0 & & \\
 & & & & \downarrow & & \downarrow & & \\
 & & & & \bigoplus \mathbb{Z}[E_i] & \xrightarrow{=} & \bigoplus \mathbb{Z}[E_i] & & \\
 & & & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & M & \longrightarrow & M' & \xrightarrow{U} & \mathrm{Pic}(X) & \longrightarrow & 0 \\
 & & \downarrow{=} & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & M & \longrightarrow & M'' & \dashrightarrow & Ab(G) & & \\
 & & & & \downarrow & & \downarrow & & \\
 & & & & 0 & & 0 & &
\end{array}
$$

The dotted arrow from M'' to $Ab(G)$ is unique and makes the diagram commute, it is surjective and the lower horizontal sequence is exact. Moreover, all these lattice homomorphisms correspond to homomorphisms of considered fans. Finally, it follows that the lower horizontal sequence gives a description of X_{Δ} as the (toric) quotient $\mathbb{C}^3/Ab(G)$. □

The situation described by Lemma 4.2.7 above is the right-hand side part of the following diagram. We would like to understand its left-hand side part, or, more precisely, prove that the image of two gray arrows, which are restrictions of respective morphisms from the right-hand side of the diagram, is isomorphic to the singularity $\mathbb{C}^2/G$, embedded in $\mathbb{C}^3/Ab(G)$. It follows then that the good categorical quotient (see Definition 2.2.1) $\mathrm{Spec}(\mathrm{Cox}(X))/\!\!/T$ is $\mathbb{C}^2/G$.



The proof presented below might seem to be just a technical argument, but in fact it is strongly connected to investigating the relation between the Cox rings of a resolution and of the quotient singularity, which is one of the most important ideas of this work, developed in section 5.2.

We first consider the (good categorical) quotient $\mathbb{C}^3 \xrightarrow{/Ab(G)} X_\Delta$ and prove that the image of S and Y (or W) in X_Δ can be described as a quotient by $Ab(G)$ of a hypersurface in $\mathbb{C}^3$, given by an equation semi-invariant with respect to the action of $Ab(G)$ (i.e. its eigenvector). Our argument is related to methods used in chapter 5. Another way of proving this statement would be to analyze lifting of semi-invariants of $Ab(G)$ through $\mathbb{C}^{n+3} \xrightarrow{/\!\!/T} X_\Delta$, however, it also requires some work and the result is not immediate. The second step of our proof, contained in Lemma 4.2.9, is the observation that the quotient of considered hypersurface in $\mathbb{C}^3$ by the action of $Ab(G)$ is indeed $\mathbb{C}^2/G$.

First of all, we describe the situation in the toric setting in more detail and introduce a variety $X_\Gamma \cap S$, which will be used in the further part of the argument. Since Δ is simplicial, X_Δ is a quotient of $\mathbb{C}^3$ by a finite group action. Let $N'' \simeq \mathbb{Z}^3$ and Γ be the fan consisting of the positive octant in N'' and all its faces.

$$\begin{array}{ccc} N' & \xrightarrow{K} & N \\ \uparrow{\scriptstyle\eta} & \searrow^{\pi} & \downarrow{\scriptstyle id_N} \\ N'' & \xrightarrow[\omega]{} & N \end{array} \qquad \begin{array}{ccc} \Sigma' & \xrightarrow{K} & \Sigma \\ \uparrow{\scriptstyle\eta} & \searrow^{\pi} & \downarrow{\scriptstyle id_N} \\ \Gamma & \xrightarrow[\omega]{} & \Delta \end{array} \tag{4.2.2.1}$$

Then $\omega\colon N'' \to N$ which sends the standard basis to the rays of Δ is the toric description of this quotient map. But the embedding $\eta\colon N'' \hookrightarrow N'$, which maps the standard basis to the rays corresponding to variables x_1, x_2 and x_3, commutes with π and ω, i.e. the lower triangle in the diagram 4.2.2.1 is commutative.

In coordinates corresponding to the standard bases η is just the embedding of $\mathbb{C}^3$ by x_1, x_2, x_3 to the subspace defined by $y_0 = 1$ and $y_{i,j} = 1$ for all possible i, j. Therefore the restriction of S to $\mathbb{C}^3 \simeq X_\Gamma \subset X_{\Sigma'} \simeq \mathbb{C}^{n+3}$ with coordinates x_1, x_2, x_3 is given by the equation obtained from the equation of S by leaving x_1, x_2, x_2 without change and substituting 1 for all other variables:

$$x_1^{p_1} + x_2^{p_2} + x_3^{p_3} = 0. \tag{4.2.2.2}$$

Recall that p_i is the last entry of the vector α_i orthogonal to the i-th branch (see Lemma 4.1.6), appearing also in the description of the minimal resolution by Hirzebruch-Jung continuous fractions and in the formula for the outer rays of Σ, see Lemma 4.1.17. (Note that this is essentially the same as in the toric localization procedure Proposition 2.2.6, just under a bit different assumptions.)

Lemma 4.2.8. *The images of $X_\Gamma \cap S$, S and W in X_Δ (under morphisms corresponding to ω and π respectively) are equal.*

Proof. Take any point

$$p = (y_0, y_{1,1}, \ldots, y_{1,n_1}, x_1, y_{2,1}, \ldots, y_{2,n_2}, x_2, y_{3,1}, \ldots, y_{3,n_3}, x_3) \in W.$$

First assume that $y_0 = 0$ or some $y_{i,j} = 0$. But π forgets rays of Σ' corresponding to these coordinates, so whole T-orbits given by these equalities are mapped to 0. Hence also closures of these orbits are mapped to 0, and we are left with the situation when all coordinates $y_{i,j}$ and y_0 are nonzero. But the orbit of such a point p contains a point of $S \cap X_\Gamma$. It is sufficient to find $\underline{t} = (t_0, \ldots, t_{n-1}) \in t$ such that $\underline{t}^{u_k}$, where u_k is the k-th column of the extended intersection matrix U, is the inverse of the k-th coordinate of p, excluding the coordinates corresponding to x_1, x_2, x_3. Such a set of equations has a solution if only the columns of the intersection matrix U_0 are linearly independent, which is true. Hence each orbit in W is mapped to a point of the image of $S \cap X_\Gamma$ in X_Δ and the other inclusion is obvious. □

Therefore from now on we consider the image of the restriction of S to X_Γ in X_Δ instead of the image of W or S.

Lemma 4.2.9. *The image of $S \cap X_\Gamma$ in X_Δ is isomorphic to $\mathbb{C}^2/G$.*

Proof. From the table in [Bri68, Satz 2.11] we can read out the parameters of the minimal resolution of $\mathbb{C}^2/G$, i.e. the invariant $\langle d; p_1, q_1; p_2, q_2; p_3, q_3 \rangle$ describing the Hirzebruch-Jung continuous fractions associated with the resolution. Substituting values of p_i into equation (4.2.2.2) we obtain the following equations of $S \cap X_\Gamma$:

$$\begin{array}{lll} BD_{n,m} & : & x_1^2 + x_2^2 + x_3^n = 0 \\ BT_m & : & x_1^2 + x_2^3 + x_3^3 = 0 \\ BO_m & : & x_1^2 + x_2^3 + x_3^4 = 0 \\ BI_m & : & x_1^2 + x_2^3 + x_3^5 = 0 \end{array}$$

Comparing with Lemma 3.2.4 and [Rei, Table 1] we see that for a group G the equation above is just an equation of an embedding of the quotient singularity $\mathbb{C}^2/[G,G]$ in $\mathbb{C}^3$. (For $G = BT_m$, i.e. $[G,G] = BD_2$, the equation is most often given in the form $x_1^2 + x_2^3 + x_2x_3^2 = 0$, but it is the same up to a change of coordinates.)
Recall that X_Δ is a quotient of $\mathbb{C}^3$ by an action of a finite group $J = \operatorname{coker}\omega$. The image of W in X_Δ is then the quotient of $S \cap X_\Gamma$ by J. We can write ω in the standard basis using the matrix with the outer vectors of Σ as columns. For all considered groups it is easy to check that J is isomorphic to the abelianization of G. One has to use again the numbers p_i, q_i associated with the minimal resolution (from [Bri68, Satz 2.11]) to write down the outer rays and describe J, and then compare with the abelianizations of small subgroups of $GL(2,\mathbb{C})$ computed in Corollary 3.2.5.
Our aim is now to prove that the the quotient $(S \cap X_\Gamma)/J$ is isomorphic to $\mathbb{C}^2/G \simeq (\mathbb{C}^2/[G,G])/Ab(G)$. Thus we have to argue that the isomorphism between $S \cap X_\Gamma$ and $\mathbb{C}^2/[G,G]$ is equivariant with respect to considered actions of $J \simeq Ab(G)$. We do this by comparing the actions on the coordinate rings: the action of generators of J on the chosen coordinates of X_Γ turn out to be identical to the action of the corresponding generators of $Ab(G)$ on the $[G,G]$-invariants which satisfy the equation of $S \cap X_\Gamma$.
The action of $Ab(G)$ on the invariants of $[G,G]$ is quite easy to describe. We sketch the idea here and give an example of computations below. Sets of generators of $\mathbb{C}[x,y]^{[G,G]}$ for small subgroups $G \subset GL(2,\mathbb{C})$ are listed for example in [DZ93]. However, not every (minimal) generating set can be used here. We need a set of generators which are eigenvectors of the action of $Ab(G)$, because coordinates of X_Γ satisfy this condition. For most types of groups the invariants given in [DZ93] are eigenvectors of $Ab(G)$ (and, in fact, there is no other choice of minimal generating set), only in the case of BT_m, where the commutator subgroup is BD_2, one has to take suitable linear combinations of $x^4 + y^4$ and x^2y^2. (It is worth noting that we speak in more detail of $[G,G]$-invariants which are eigenvectors of the action of $Ab(G)$ in section 5.2; moreover, we list them in Example 5.3.2.) Finally, we take some representatives of the generating classes of $Ab(G)$ and determine their action on the chosen invariants by an explicit computation.
To describe the action of $J \simeq Ab(G)$ on variables x_1, x_2, x_3 corresponding to the rays of Γ we take a vector of N representing a generator and evaluate it on the dual characters to the rays of Δ, which are

$$\begin{aligned} u_1 &= \frac{1}{r}(p_1p_2, q_1p_2, q_2p_1), \\ u_2 &= \frac{1}{r}(p_1p_3, q_1p_3, dp_1p_3 - p_1q_3 - q_1p_3), \\ u_3 &= \frac{1}{r}(p_2p_3, dp_2p_3 - p_2q_3 - q_2p_3, q_2p_3), \end{aligned}$$

where

$$r = dp_1p_2p_3 - q_1p_2p_3 - p_1q_2p_3 - p_1p_2q_3$$

is the order of J (equal to the determinant of the matrix which has the outer rays as columns).

In all the cases of cyclic abelianizations one can take as a generator of J one of the standard basis vectors. In the only non-cyclic case ($BD_{n,m}$ for even n) the generators can be chosen for example $(0, 1, 0)$ and $(-1, 1, 1)$. However, these generators do not necessarily give the same action of $Ab(G)$ on the chosen $[G, G]$-invariants, so one has to find a suitable power of a generator to get exactly the same numbers. We have checked that such generators can be found in all the cases. As all the computations are very similar, we end the proof by presenting only a chosen case in detail.

Let us look at the action of $G = BO_m$. Recall that we have to assume $(m, 6) = 1$. First, the generators of the invariants of $[G, G] = BT$ are

$$\begin{aligned} w_1 &= x^5y - xy^5, \\ w_2 &= x^8 + 14x^4y^4 + y^8, \\ w_3 &= x^{12} - 33x^8y^4 - 33x^4y^8 + y^{12}, \end{aligned}$$

which, up to some constants, satisfy the relation $w_1^4 + w_2^3 + w_3^2 = 0$. As stated in Corollary 3.2.5, $Ab(G) \simeq \mathbb{Z}_{2m}$ is generated by $g = \varepsilon_{2m} \cdot \mathrm{diag}(\varepsilon_8, \varepsilon_8^{-1})$. The action on the $[G, G]$-invariants is

$$\begin{aligned} g \cdot w_1 &= -\varepsilon_{2m}^6 \cdot w_1 = \varepsilon_{2m}^{m+6} \cdot w_1, \\ g \cdot w_2 &= \varepsilon_{2m}^8 \cdot w_2, \\ g \cdot w_3 &= -\varepsilon_{2m}^{12} \cdot w_3 = \varepsilon_{2m}^{m+12} \cdot w_3. \end{aligned}$$

Now look at the action of J. Take $v = (0, 1, 0) \in N$. Then

$$u_1(v) = \frac{3}{r} = \frac{3}{2m}.$$

The equality $r = 2m$ can be obtained directly from the parameters of resolutions given in [Bri68, Satz 2.11]. As m is not divisible by 3, v is of order $2m$ in J, so it is a generator. The weights of its action are

$$\begin{aligned} 2m \cdot u_1(v) &= 3, \\ 2m \cdot u_2(v) &= 4, \\ 2m \cdot u_3(v) &= 12d - 3q_3 - 4q_2 = m + 6. \end{aligned}$$

Take $v' = (0, m + 2, 0) \in N$, which is also a generator of J because m is odd. Then

$$\begin{aligned} 2m \cdot u_1(v') &= 3(m + 2) \equiv m + 6 \mod 2m, \\ 2m \cdot u_2(v') &= 4(m + 2) \equiv 8 \mod 2m, \\ 2m \cdot u_3(v') &= (m + 6)(m + 2) = m^2 + 12 + 8m \equiv m + 12 \mod 2m, \end{aligned}$$

hence both considered actions are the same. □

The observations made above are summarized in the following statement.

Proposition 4.2.10. *The good categorical quotient* $\mathbb{C}^{n+3} \xrightarrow{/\!\!/T} \mathbb{C}^3/Ab(G)$ *restricts to the good categorical quotient* $S \xrightarrow{/\!\!/T} \mathbb{C}^2/G$*, which induces a birational morphism from* $Y = W/T$ *onto* $\mathbb{C}^2/G$.

Corollary 4.2.11. *The quotient* $Y = W/T$ *is a resolution of the singularity* $\mathbb{C}^2/G$.

Proof. The birational morphism from Y to $\mathbb{C}^2/G$ constructed above is induced by the fan morphism from Σ to the fan Δ, which consists of a cone spanned by the outer rays of Σ and all its faces. This homomorphism is induced by the identity on the lattice N, it is just forgetting about all the rays except the outer ones. Therefore it gives the identity on the orbits corresponding to all the faces of the maximal cone of Δ, i.e. on $(\mathbb{C}^2/G) \setminus \{0\}$. □

4.2.3 Minimality

We prove that $Y = W/T$ is in fact the minimal resolution of the considered quotient singularity. Moreover, we explain how the class groups of Y and X_Σ are related, which will be needed in the proof of Proposition 4.3.2.
By $\rho_{i,j}$ for $i = 1, 2, 3$ and $1 \leq j \leq n_i + 1$ we denote the j-th ray on the i-th branch in the fan of Σ. The central ray is denoted ρ_0.

Notation 4.2.12. Let $D_{i,j}$ be the torus invariant divisor in X_Σ corresponding to $\rho_{i,j}$ and D_0 corresponds to ρ_0. Then $C_0 = Y \cap D_0$ and $C_{i,j} = Y \cap D_{i,j}$ for $j \leq n_i$ are the exceptional curves of the map from Y to $\mathbb{C}^2/G \subset X_\Delta$ constructed in Proposition 4.2.10. Note that the curve $C_{i,n_i+1} = Y \cap D_{i,n_i+1}$ is not exceptional.

First we show that for any ray $\rho_{i,j}$ one can choose a (non-unique) simplicial fan Σ such that $D_{i,j}$ is isomorphic to a Hirzebruch surface (described in terms of toric geometry in 2.1.6).

Lemma 4.2.13. *Let* Σ *be a fan satisfying conditions in Notation 4.1.20 and such that each of* $\rho_{i,j-1}$, $\rho_{i,j}$ *and* $\rho_{i,j+1}$ *lies in 2-dimensional faces with the first rays on two other branches (if* $j = 0$ *we put* $\rho_{i,j-1} = \rho_0$*), see Fig. 4.2. Then* $D_{i,j}$ *is isomorphic to the Hirzebruch surface* $F_{(\gamma_i)_{j+1}}$*, where* $(\gamma_i)_{j+1}$ *is the* $(j+1)$*-st entry of the vector* $\gamma_i \in \ker A''_i$ *from formula (4.1.1.1).*

Proof. Note that such a fan Σ exists for any $\rho_{i,j}$. Fig. 4.2 shows a section of the cone spanned by the outer rays of Σ. The four gray cones are the cones containing $\rho_{i,j}$, we will prove that their projection along $\rho_{i,j}$ onto a plane give the fan of $F_{(\gamma_i)_{j+1}}$.
We give the proof in the case where $\rho_{i,j}$ is from the third branch, i.e. $i = 3$ and $\rho_{3,j} = (c, -d, -d)$ for some $c, d \in \mathbb{N}$. The remaining cases can be reduced to this one by a lattice automorphism. Let $\rho_{3,j-1} = (a, -b, -b)$ and $\rho_{3,j+j} = (e, -f, -f)$, where a, b, e, f are positive integers. All cones of Σ containing $\rho_{3,j}$ are spanned by one of these vectors and one of $\rho_{1,1} = (0, 1, 0)$, $\rho_{2,1} = (0, 0, 1)$.
Let $\eta_1 = \rho_{2,1} - \rho_{3,j} = (-c, d, d+1)$ and $\eta_2 = \rho_{3,j-1} - \rho_{3,j} = (a-c, d-b, d-b)$. By [CLS11, Proposition 3.2.7] it is sufficient to prove that projections along $\rho_{3,j}$ onto the plane spanned by η_1 and η_2 of these two vectors and $\zeta_1 = \rho_{1,1} - \rho_{3,j} =$

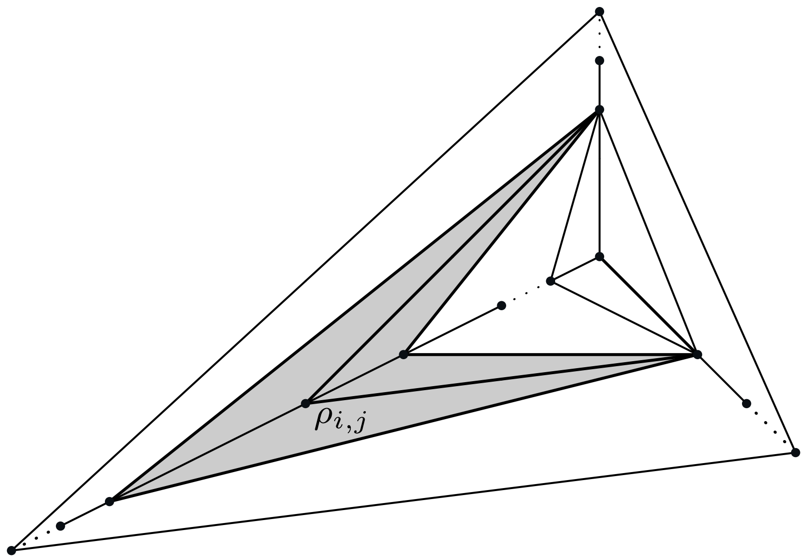


Figure 4.2: Cones containing $\rho_{i,j}$ in a fan where $D_{i,j}$ is a Hirzebruch surface

$(-c, d+1, d)$, $\zeta_2 = \rho_{3,j+1} - \rho_{3,j} = (e-c, d-f, d-f)$ are the rays of the fan of $F_{(\gamma_i)_{j+1}}$.
Recall that by Lemma 4.1.21 (3) cones $\sigma(\rho_{3,j-1}, \rho_{3,j})$ and $\sigma(\rho_{3,j}, \rho_{3,j})$ are smooth, so we have

$$-ad + bc = -1 = -cf + de.$$

It follows that

$$\zeta_2 + \eta_2 = (e + a - 2c, 2d - b - f, 2d - b - f) = \frac{b + f - 2d}{d}(c, -d, -d),$$

that is ζ_2 is projected to $-\eta_2$. We now show that ζ_1 is projected to $-\eta_1 + r\eta_2$ and that $r = (\gamma_3)_j$. Because

$$\zeta_1 + \eta_1 - r\eta_2 = -2\rho_{3,j} + (0, 1, 1) - r(a - c, d - b, d - b),$$

it is enough to find r such that $(0, 1, 1) - r(a - c, d - b, d - b) = k\rho_{3,j}$ for some $k \in \mathbb{R}$. But then

$$\frac{-r(a-c)}{c} = k = \frac{1 - r(d-b)}{-d},$$

hence

$$c = r(ad - bc) = r.$$

By Notation 4.1.10 the first coordinate of $\rho_{3,j}$ is $(\gamma_3)_{j+1}$, which finishes the proof. □

Proposition 4.2.14. *Y is the minimal resolution of $\mathbb{C}^2/G$. Moreover, $\mathrm{Cl}(Y)$ is generated by restrictions to Y of divisors in X_Σ which are invariant under the action of the big torus of this variety. The intersection numbers of these divisors and the exceptional curves are the entries of the extended intersection matrix U.*

Proof. By Lemma 4.2.3, W and hence also Y does not depend on the choice of Σ. Moreover, $\mathrm{Cl}(X_\Sigma)$ does not depend on the choice of Σ, since all considered fans have the same set of rays. Thus we can investigate each exceptional curve $C_{i,j}$ in a suitably chosen fan, in which $D_{i,j}$ is isomorphic to the Hirzebruch surface $F_{(\gamma_i)_{j+1}}$, as in Lemma 4.2.13.

One can compute local equation of Y on affine pieces of X_Σ using the toric localization, see Proposition 2.2.6. In local coordinates it is easy to check that $C_{i,j} \cdot C_{i,j+1} = 1$ and $C_0 \cdot C_{i,1} = 1$ in Y for all admissible i, j: we just obtain that they intersect transversally in a point. We skip the details and move to computing $C_{i,j} \cdot C_{i,j}$ in Y.

Look at $D_{i,j} \simeq F_{(\gamma_i)_{j+1}}$ as at a $\mathbb{P}^1$-fibration over $\mathbb{P}^1$, the structure of which is determined by cones in Σ containing $\rho_{i,j}$. Passing to local coordinates again, we check that $C_{i,j}$ is a fibre of this fibration. However, it is not one of the fibres which are torus invariant curves in X_Σ and correspond to 2-dimensional faces joining $\rho_{i,j}$ with the first rays on other branches. We see in local coordinates that Y intersects $D_{i,j}$ transversally in $C_{i,j}$.

Let ι and κ denote the embedding of Y and $D_{i,j}$ in X_Σ respectively. By the projection formula

$$\iota_*(\iota^*\mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot C_{i,j}) = \mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot \iota_* C_{i,j}.$$

Since $\iota^*\mathcal{O}_{X_\Sigma}(D_{i,j})$ is just $D_{i,j} \cap Y = C_{i,j}$, the left hand side is just the self-intersection number of $C_{i,j}$ in Y. And the right hand side is $D_{i,j} \cdot C_{i,j}$ in X_Σ.

Let $C'_{i,j}$ be one of the fibres in $D_{i,j} \simeq F_{(\gamma_i)_{j+1}}$ which is a torus invariant curve in X_Σ. Assume that it corresponds to the face $\sigma(\rho_{i,j}, \rho_{k,1})$. Then, because $C_{i,j}$ and $C'_{i,j}$ are numerically equivalent in $D_{i,j}$,

$$\begin{aligned}\mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot \iota_* C_{i,j} = \mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot \kappa_* C_{i,j} = \kappa_*(\kappa^*\mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot C_{i,j}) = \\ = \kappa_*(\kappa^*\mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot C'_{i,j}) = \mathcal{O}_{X_\Sigma}(D_{i,j}) \cdot \kappa_* C'_{i,j}.\end{aligned}$$

Summing up, instead of the self-intersection number of $C_{i,j}$ in Y we compute $D_{i,j} \cdot C'_{i,j}$ in X_Σ, which can be done in the toric setting.

We use the formula for toric intersection product from [CLS11, Prop. 6.3.8]. Because Σ is simplicial, X_Σ is $\mathbb{Q}$-factorial (see Proposition 2.1.10). Hence some multiple of $D_{i,j}$ is Cartier. Then $D_{i,j}$ can be described by a set $\{m_\sigma \colon \sigma \in \Sigma_{max}\}$, almost as in Proposition 2.1.9, but $m_\sigma \in \mathbb{Q} \cdot M$. Let m_1 and m_2 be the elements of this set corresponding to $\sigma(\rho_{k,1}, \rho_{i,j-1}, \rho_{i,j})$ and $\sigma(\rho_{k,1}, \rho_{i,j}, \rho_{i,j+1})$ respectively. Then they satisfy

$$\langle m_1, \rho_{i,j}\rangle = \langle m_2, \rho_{i,j}\rangle = -1, \ \langle m_1, \rho_{i,j-1}\rangle = \langle m_2, \rho_{i,j+1}\rangle = \langle m_1, \rho_{k,1}\rangle = \langle m_2, \rho_{k,1}\rangle = 0.$$

By [CLS11, Prop. 6.3.8] we have

$$D_{i,j} \cdot C'_{i,j} = \langle m_1 - m_2, \rho_{i,j+1}\rangle.$$

We show the computations in the case where $i = 3$ and $k = 1$, other cases can be reduced to this one by applying a lattice automorphism. For $1 \le p \le n_3 + 1$ we have

$$\rho_{1,1} = (0, a, 0), \quad \rho_{3,p} = (b_p, c_p, c_p).$$

Moreover, by part 3. of Lemma 4.1.14 adjacent rays on each branch form a basis of the restriction of N to the subspace spanned by them, so $b_p c_{p-1} - b_{p-1} c_p = 1$ (the arrangement is such that this determinant is positive). Hence

$$m_1 = (c_{j-1}, 0, -b_{j-1}), \quad m_2 = (-c_{j+1}, 0, b_{j+1})$$

and thus

$$D_{3,j} \cdot C'_{3,j} = \langle m_1 - m_2, \rho_{i,j+1} \rangle = \langle m_1, \rho_{i,j+1} \rangle = c_{j-1} b_{j+1} - b_{j-1} c_{j+1}.$$

Since b_p, c_p are entries of vectors $\overline{\gamma_3}$ and $-\alpha_3$ in the kernel of A''_3 (see Lemma 4.1.9 and its proof), they satisfy recursive relations

$$b_{p+1} = -(a_{3,p} b_p + b_{p-1}) \text{ and } c_{p+1} = -(a_{3,p} c_p + c_{p-1})$$

with $b_0 = 1$, $b_1 = d$, $c_0 = 0$, $c_1 = 1$. Hence we check that

$$c_{j-1} b_{j+1} - b_{j-1} c_{j+1} = -c_{j-1}(a_{3,j} b_j + b_{j-1}) + b_{j-1}(a_{3,j} c_j + c_{j-1}) = \\ = -a_{3,j}(c_{j-1} b_j - b_{j-1} c_j) = -a_{3,j},$$

and, summarizing,

$$C_{i,j} \cdot_S C_{i,j} = D_{3,j} \cdot_{X_\Sigma} C'_{3,j} = -a_{i,j}.$$

In a very similar way we compute $C_0 \cdot C_0$, which is equal to the intersection number of D_0 with the curve in X_Σ corresponding to one of the cones $\sigma(\rho_0, \rho_{i,1})$. Thus we obtain

$$C_0 \cdot C_0 = -d.$$

In order to compute the intersection number of C_{i,n_i+1}, which is not exceptional, with C_{i,n_i} we consider the fan where ρ_{i,n_i} and ρ_{i,n_i+1} form (smooth) cones with the first rays on two other branches. Passing to local coordinates we get the result

$$\mathbb{C}_{i,n_1+1} \cdot C_{i,n_i} = 1.$$

Therefore the intersection numbers of the exceptional curves C_0 and $C_{i,j}$ for $j \le n_i$ with the divisors C_0, $C_{i,j}$ for $j \le n_i + 1$ in Y are just the entries of the extended intersection matrix U. In particular, Y is the minimal resolution of $\mathbb{C}^2/G$.
To prove that the restrictions of the torus invariant divisors in X_Σ to Y generate $\mathrm{Cl}(Y)$ it suffices to show that the subgroup generated by these divisors contains duals of the exceptional curves. Since their intersection numbers are the entries of U, this is equivalent to the fact that the system of equations given by the rows of U with the constant terms such that one is 1 and the remaining are 0 has an integral solution. And such solutions can be easily constructed using the methods as in the proof of Lemma 4.1.9. □

4.3 The spectrum of the Cox ring

The aim of this section is to finish the proof of Theorem 4.3.3, which states that the hypersurface $S \subset \mathbb{C}^{n+3}$ introduced in Construction 4.1.22 is the spectrum of the Cox ring of the minimal resolution X of a surface quotient singularity $\mathbb{C}^2/G$. Our argument is based on Theorem 3.5.7, which provides a characterization of the Cox rings via Geometric Invariant Theory.
As before, we investigate S, its T-invariant open subset

$$W = S \setminus Z(\Sigma)$$

(independent of the choice of Σ) and the geometric quotient $Y = W/T$. The most difficult part of the proof is the content of the previous section, but we still need to check a few properties of these spaces to see whether the assumptions of Theorem 3.5.7 are fulfilled. Some of them are direct consequences of the observations we have already made, the remaining ones are proven below.
It is worth noting that the quotients considered here are a special case of a much more general theory of good quotients of algebraic varieties by reductive group actions, developed by Białynicki-Birula and Święcicka in a series of papers including [BBS96], which can be useful for a possible generalization of our results.
The first property is the strong stability of the action of T on W (see Definition 3.5.6). Then, in Proposition 4.3.2, we prove the T-factoriality of S (see Definition 3.5.5).

Proposition 4.3.1. *The action of T on W is strongly stable.*

Proof. We take $W' := W$. Then, obviously, W' is T-invariant and the codimension of its complement in W is ≥ 2. Also, by Remark 4.2.1 all the orbits of T in W are closed. Finally, in Lemma 4.2.5 it is proven that T acts freely on W, which finishes the proof. □

Proposition 4.3.2. *The hypersurface S is T-factorial.*

Proof. First notice that every T-invariant Weil divisor in S is a pull-back of a divisor in $Y = W/T$. This is because of dimension reasons: T is an n-dimensional torus acting freely on an $(n+2)$-dimensional variety W, and $S \setminus W$ is of codim ≥ 2 in S, so an invariant divisor cannot be mapped to a subset of codimension bigger than one. Hence it is sufficient to show that the pull-backs of generators of $\mathrm{Pic}(Y)$ are principal. Their equations are $\{y_{i,j} = 0\}$ or $\{x_i = 0\}$, where the coordinates on $\mathbb{C}^{n+3} \supset S$ are denoted as in Construction 4.1.22. Thus the question is whether Cartier divisors defined by these functions are not multiples of Weil divisors defined as intersections of hyperplanes $\{y_{i,j} = 0\}$ and $\{x_i = 0\}$ with S. Thus we have to check whether valuations corresponding to local rings of S are 1 on $y_{i,j}$ and x_i.
The argument is the same for all functions x_i and $y_{i,j}$, so we may choose x_1 and check that it is not in the square of the maximal ideal of the localization of $\mathbb{C}[S]$ in a generic point of $\{x_1 = 0\} \cap S$. As S is given by the equation

$$\sum_{i=1,2,3} y_{i,1}^{(\alpha_i)_1} \cdots y_{i,n_i}^{(\alpha_i)_{n_i}} \cdot x_i^{(\alpha_i)_{n_i+1}},$$

the ideal with respect to which we localize contains

$$y_{2,1}^{(\alpha_2)_1} \cdots y_{2,n_2}^{(\alpha_2)_{n_2}} x_2^{(\alpha_2)_{n_2+1}} + y_{3,1}^{(\alpha_3)_1} \cdots y_{3,n_3}^{(\alpha_3)_{n_3}} x_3^{(\alpha_3)_{n_3+1}}.$$

However, it is irreducible, so we cannot obtain from it any elements of the ideal dividing x_1, hence x_1 is a generator of the maximal ideal of the localization. □

We are ready to complete the proof of the main theorem of this section.

Theorem 4.3.3. *Let X be the minimal resolution of a surface quotient singularity $\mathbb{C}^2/G$. If S is as defined in Construction 4.1.22, then $S \simeq \operatorname{Spec}(\operatorname{Cox}(X))$.*

Proof. S is a hypersurface in a smooth variety and its set of singular points has codimension ≥ 2 (if its Jacobian matrix is zero in a point, then at least three coordinates are zero), so it is a normal variety by the Serre's criterion (see e.g. [Mat89, Thm 23.8]). Moreover, every invertible function on S is constant. To see this, first observe that the affine space V described by conditions $y_{1,0} = y_{2,0} = y_{3,0} = 0$ is contained in S (given by equation 4.1.3.1). Since on an affine space all invertible functions are constant, the restriction of such a function on S to V is constant, in particular equal to the value of this function in 0. Take any point

$$p = (v_0, u_1, v_{1,1}, \ldots, v_{1,n_1+1}, u_2, v_{2,1}, \ldots, v_{2,n_2+1}, u_3, v_{3,1}, \ldots, v_{3,n_3+1}) \in S.$$

If we show an affine space contained is S, passing through p and intersecting V, we obtain that a value of any invertible rational function in p is equal to its value in 0. Remember that variables $y_{1,1}$, $y_{2,1}$, $y_{3,1}$ appear in the equation of S with exponent 1 (see Remark 4.1.23). Thus the equations $x_i = u_i$, $y_0 = v_0$, $y_{i,j} = v_{i,j}$ for all $i = 1, 2, 3$, $j = 0$ and $j > 1$ together with the equation of S determine a plane in S: the equation of S transforms to $q_1 y_{1,1} + q_2 y_{2,1} + q_3 y_{3,1} = 0$ for suitable $q_1, q_2, q_3 \in \mathbb{C}$. It passes through p and intersects V as desired.
By Proposition 4.3.2 we know that S is T-factorial. Now $W \subset S$ is an open and T-invariant subset such that $\operatorname{codim}_S(S \setminus W) \geq 2$. The action of T on W admits a good quotient, as it was observed in Remark 4.2.1. Finally, by Proposition 4.3.1 this action is strongly stable. Therefore it follows from Theorem 3.5.7 that S is the spectrum of the Cox ring of X. □

Corollary 4.3.4. *The Cox ring of the minimal resolution of a surface quotient singularity is a finitely generated $\mathbb{C}$-algebra.*

Chapter 5

Generators of the Cox ring

In this chapter we focus on investigating the relation between Cox rings of the singularity $\mathbb{C}^2/G$ and its minimal resolution X. This leads us to a description of generators of $\mathrm{Cox}(X)$ presented in a natural way as a subring of the coordinate ring of $\mathbb{C}^2/[G,G] \times T$ (see Theorem 5.2.9).
We start from statements concerning the structure of the invariant ring $\mathbb{C}^{[G,G]}$ and the Cox ring of a quotient singularity (in arbitrary dimension). After that the main result of this part, Theorem 5.2.9, is proven, and in section 5.3 we give a few examples of the construction of an embedding

$$\mathrm{Cox}(X) \hookrightarrow \mathbb{C}[a,b]^{[G,G]} \otimes \mathbb{C}[T].$$

We expect that the ideas sketched in this chapter work in a more general setting, and that they will form a basis for the extension of this work to higher dimensional quotient singularities, at least for some specific classes of groups, in particular 4-dimensional symplectic quotient singularities. The work presented here will be continued and developed in a forthcoming paper [DBW13].

5.1 The Cox ring of a quotient singularity

Consider a linear action of $G \subset GL(n,\mathbb{C})$ on an affine space $V \simeq \mathbb{C}^n$ and on $\mathbb{C}[V]$. Look at the induced action of $Ab(G)$ on the ring $\mathbb{C}[V]^{[G,G]}$ of invariants of the commutator. Note that $\mathbb{C}[V]^{[G,G]}$ is a $\mathbb{C}[V]^G$-module and that the character group of G satisfies $G^\vee = Ab(G)^\vee \simeq Ab(G)$. Moreover, by [Ben93, Thm 3.9.2] we have $\mathrm{Cl}(V/G) \simeq Ab(G)$, see also Proposition 3.4.8. We are interested in relative invariants of the action of G, i.e. regular or rational functions on V which are eigenvectors of G and the action on such a function is the multiplication by values of a character μ of G (see [Ben93, Sect. 1.1], or a more general definition in [Sta79, Sect. 1], where μ is not required to be a linear character). In particular, we need to consider these relative invariants which are contained in $\mathbb{C}[V]^{[G,G]}$.

Definition 5.1.1. By $\mathbb{C}[V]^G_\mu$ we denote the eigenspace of the action of $Ab(G)$ on $\mathbb{C}[V]^{[G,G]}$ corresponding to a linear character $\mu \in G^\vee$, i.e. a submodule (over $\mathbb{C}[V]^G$)

consisting of all $f \in \mathbb{C}[V]^{[G,G]}$ such that for any $g \in Ab(G)$ we have

$$g(f) = \mu(g)f.$$

In general, $\mathbb{C}[V]$ decomposes as a direct sum of its $\mathbb{C}[V]^G$-submodules of relative invariants (see e.g. [Sta79, Sect. 1.1]). The following lemma describes restriction of this decomposition to $\mathbb{C}[V]^{[G,G]}$. We present the proof to get more insight into the behavior of relative invariants.

Lemma 5.1.2. *The ring of invariants $\mathbb{C}[V]^{[G,G]}$ decomposes as a sum of eigenspaces of $Ab(G)$ associated with all characters of G*

$$\mathbb{C}[V]^{[G,G]} = \bigoplus_{\mu \in G^\vee} \mathbb{C}[V]^G_\mu.$$

Each of these eigenspaces is a $\mathbb{C}[V]^G$-module of rank 1, associated with a class in $\mathrm{Cl}(V/G) \simeq Ab(G)$.

Proof. First look at the sequence of ring inclusions and the corresponding inclusions of fields of fractions

$$\mathbb{C}[V]^G \subset \mathbb{C}[V]^{[G,G]} \subset \mathbb{C}[V], \qquad \mathbb{C}(V)^G \subset \mathbb{C}(V)^{[G,G]} \subset \mathbb{C}(V).$$

Note that $\mathbb{C}(V)^G$ means both the field of fractions of $\mathbb{C}[V]^G$ and the subfield of invariants of the induced action of G on $\mathbb{C}(V)$. This is because if f/h is a G-invariant fraction then we can multiply numerator and denominator by $\prod_{g \in G \setminus \{1\}} g(f)$ to obtain an element of the field of fractions of $\mathbb{C}[V]^G$ (we use the assumption that G is finite).
Consider $\mathbb{C}(V)$ as a Galois extension of $\mathbb{C}(V)^G$ with the Galois group G (see e.g. [Ben93, Prop. 1.1.1]). Then $\mathbb{C}(V)^{[G,G]}$ corresponds to a normal subgroup of G, so $\mathbb{C}(V)^G \subset \mathbb{C}(V)^{[G,G]}$ is also Galois with the automorphism group $G/[G,G] = Ab(G)$. By the normal basis theorem there exists $\alpha \in \mathbb{C}(V)^{[G,G]}$ such that $\mathbb{C}(V)^{[G,G]}$ is spanned over $\mathbb{C}(V)^G$ by the orbit $\{g(\alpha) \colon g \in Ab(G)\}$. This basis endowed with the action of $Ab(G)$ is isomorphic to $Ab(G)$ acting on itself by multiplication (see Lemma 1.3.1), which means that $\mathbb{C}(V)^{[G,G]}$ is the regular representation of $Ab(G)$. Hence it splits into the sum of all irreducible representations of $Ab(G)$, which are one-dimensional since $Ab(G)$ is abelian, and each of them appears once in the decomposition (see Lemma 1.3.3):

$$\mathbb{C}(V)^{[G,G]} = \bigoplus_{\mu \in Ab(G)^\vee} \mathbb{C}(V)^G_\mu.$$

It remains to prove that $\mathbb{C}[V]^{[G,G]}$ is a direct sum of $\mathbb{C}[V]^G_\mu = \mathbb{C}(V)^G_\mu \cap \mathbb{C}[V]^{[G,G]}$. Every $f \in \mathbb{C}[V]^{[G,G]}$ can be written (uniquely) as a sum

$$f = \sum_{\mu \in Ab(G)^\vee} \frac{v_\mu}{w_\mu}$$

where $v_\mu/w_\mu \in \mathbb{C}(V)^G_\mu$. We have to show that $v_\mu/w_\mu \in \mathbb{C}[V]^{[G,G]}$. Let $Ab(G) = \{g_1, \ldots, g_k\}$ and denote the rows of the character table of $Ab(G)$ by $c_1, \ldots, c_k \in (\mathbb{C}^*)^k$ (i.e. $(c_i)_j = \mu_i(g_j)$). Let $\langle c_i, c_j\rangle = \sum_{s=1,\ldots,k} \overline{(c_i)_s}(c_j)_s$. We use the orthogonality of characters

$$\langle c_i, c_i\rangle = |G|, \qquad \langle c_i, c_j\rangle = 0 \text{ for } i \neq j.$$

The image of f under $\sum_{j=1,\ldots,k} \overline{(c_i)_j} g_j$ is obviously an element of $\mathbb{C}[V]^{[G,G]}$. But for its part corresponding to the character μ_m we obtain

$$\sum_{j=1,\ldots,k} \overline{(c_i)_j} g_j(\frac{v_{\mu_m}}{w_{\mu_m}}) = \sum_{j=1,\ldots,k} \overline{(c_i)_j}(c_m)_j \frac{v_{\mu_m}}{w_{\mu_m}} = \langle c_i, c_m\rangle \frac{v_{\mu_m}}{w_{\mu_m}} = \begin{cases} |G|\frac{v_{\mu_m}}{w_{\mu_m}} & \text{for } i = m, \\ 0, & \text{for } i \neq m. \end{cases}$$

Therefore

$$\sum_{j=1,\ldots,k} \overline{(c_i)_j} g_j(f) = \sum_{\mu \in Ab(G)^\vee} \sum_{j=1,\ldots,k} \overline{(c_i)_j} g_j(\frac{v_\mu}{w_\mu}) = |G|\frac{v_{\mu_i}}{w_{\mu_i}},$$

so $\frac{v_{\mu_i}}{w_{\mu_i}}$ is indeed a polynomial for $i = 1, \ldots, k$. □

The following proposition describes the Cox ring of a quotient singularity and explains that the embedding $\mathrm{Cox}(X) \hookrightarrow \mathbb{C}[a,b]^{[G,G]} \otimes \mathbb{C}[T]$ we are about to construct relates the Cox ring of the minimal resolution to the Cox ring of the singularity.

Proposition 5.1.3. *For a complex vector space V with an action of a finite group $G \subset GL(V, \mathbb{C})$ we have*

$$\mathrm{Cox}(V/G) \simeq \mathbb{C}[V]^{[G,G]}.$$

Note that this is the instance where the considered Cox ring is not graded by a free group, see also Remark 3.5.2.

Proof. The statement is proved in [AG10, Thm 3.1].
We sketch another proof, based on Lemma 5.1.2. To describe the module structure of $\mathrm{Cox}(V/G)$ it is sufficient to notice that rank one $\mathbb{C}[V]^G$-modules $\mathbb{C}[V]^G_\mu$ in the decomposition of $\mathbb{C}[V]^{[G,G]}$ can be identified with $\mathcal{O}(V/G)$-modules of global sections of $\mathcal{O}_{V/G}(D)$ for $D \in \mathrm{Cl}(V/G) \simeq Ab(G)$. Since the class group of V/G is a torsion group $Ab(G)$ (see Proposition 3.4.8), to define the multiplication in $\mathrm{Cox}(V/G)$ more work has to be done (see Remark 3.5.2 and [ADHL10, Sect. 4.2]). We skip this part as we will not need the exact description of the multiplication. □

5.2 Generators of $\mathrm{Cox}(X)$

Let us fix the notation. The coordinate ring of $\mathbb{C}^2$ is denoted by $\mathbb{C}[a,b]$, and of $\mathbb{C}^{n+3}$, which is the ambient space for $S = \mathrm{Spec}(\mathrm{Cox}(X))$ (see Construction 4.1.22), by

$$A = \mathbb{C}[y_0, y_{1,1}, \ldots, y_{1,n_1}, x_1, y_{2,1}, \ldots, y_{2,n_2}, x_2, y_{3,1}, \ldots, y_{3,n_3}, x_3].$$

The Picard torus $T \simeq (\mathbb{C}^*)^n$ of the minimal resolution X (see Definition 4.1.1) acts on $\mathbb{C}^{n+3}$ and on S by characters corresponding to columns of the extended intersection matrix U (see Notation 3.4.5), as described in Definition 4.1.2, and its coordinate ring is

$$\mathbb{C}[T] = \mathbb{C}[t_0^{\pm 1}, \ldots, t_{n-1}^{\pm 1}].$$

Our aim is to define a monomorphism

$$\phi\colon \mathrm{Cox}(X) \hookrightarrow \mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1}, \ldots, t_{n-1}^{\pm 1}] = \mathrm{Cox}(\mathbb{C}^2/G) \otimes \mathbb{C}[T]$$

such that composed with evaluation at $t_0 = \ldots = t_{n-1} = 1$ it gives the morphism

$$\mathrm{Cox}(X) \longrightarrow \mathrm{Cox}(V/G)$$

coming from the push-forward of divisorial sheaves. Then we view $\mathrm{Cox}(X)$ as the subring $\phi(\mathrm{Cox}(X))$ of $\mathrm{Cox}(\mathbb{C}^2/G) \otimes \mathbb{C}[T]$ and give a formula for a set of generators of this ring. But before we show the construction, let us explain how this idea works in the case of an abelian group G.

Example 5.2.1. If G is abelian, then we have

$$\mathrm{Cox}(\mathbb{C}^2/G) = \mathbb{C}[a,b]^{[G,G]} = \mathbb{C}[a,b] \quad \text{and} \quad \mathrm{Spec}(\mathrm{Cox}(X)) = \mathbb{C}^{|\Sigma(1)|},$$

where Σ is the fan of the minimal resolution X (see Remark 2.2.5). The coordinate ring of $\mathrm{Cox}(X)$ is then $\mathbb{C}[x_1, y_1, \ldots, y_n, x_2]$, where y_i correspond to components of the exceptional divisor. We define

$$\phi\colon \mathrm{Cox}(X) = \mathbb{C}[x_1, y_1, \ldots, y_n, x_2] \longrightarrow \mathbb{C}[a,b][t_0^{\pm 1}, \ldots, t_{n-1}^{\pm 1}]$$

with the formula

$$x_1 \mapsto at_0, \quad x_2 \mapsto bt_{n-1}, \quad y_1 \mapsto \chi_i(t_0, \ldots, t_{n-1}),$$

where χ_i is the character corresponding to the i-th column of the intersection matrix of X (see Remark 3.3.7 for the explanation, and the matrix is shown just under it). Since the intersection matrix of X is nonsingular (the absolute value of its determinant is just the numerator of the corresponding Hirzebruch-Jung continued fraction), ϕ is indeed a monomorphism. Its composition with the evaluation at $t_0 = \ldots = t_{n-1} = 1$ gives the toric morphism from $\mathbb{C}^{|\Sigma(1)|}$ to $\mathbb{C}^2$ coming from forgetting about rays of Σ added to the fan of $\mathbb{C}^2/G$ in the process of resolution.

From now on we assume that $G \subset GL(2,\mathbb{C})$ is a non-abelian small group. In the abelian case to define ϕ we need, apart from the characters of T, two elements of $\mathrm{Cox}(\mathbb{C}^2/G)$, which make a generating set of this ring. For non-abelian groups we have to choose three generators with special properties. They may be thought of as sections of sheaves corresponding to divisors of $\mathbb{C}^2/G$ defined by the variables x_1, x_2, x_3, associated with the ends of branches of the resolution diagram (see Section 3.4.1).

Remark 5.2.2. For all small subgroups $G \subset GL(2,\mathbb{C})$ there exist homogeneous polynomials $\sigma_1(a,b)$, $\sigma_2(a,b)$, $\sigma_3(a,b)$ invariant under the action of $[G,G]$ on $\mathbb{C}[a,b]$, which are eigenvectors of the action of $Ab(G)$ on $\mathbb{C}[a,b]^{[G,G]}$ and such that they make

a generating set of $\mathbb{C}[a,b]^{[G,G]}$ as a $\mathbb{C}$-algebra. In Example 5.3.2 we give a direct proof of existence of such generating sets, i.e. we write them down.
Moreover, such generating sets are uniquely determined up to multiplying its elements by constants. The uniqueness follows by analyzing the numbers of independent $[G,G]$-invariants in small gradations. If we look at Molien series (which can be computed for example in [GAP12]), it turns out that a few nonzero gradations of smallest degrees have rank 1 and are distributed in such a way that only one choice of $\sigma_i(a,b)$ is possible.
For most small subgroups of $GL(2,\mathbb{C})$ the homogeneity condition of $\sigma_i(a,b)$ is forced by the assumption that this polynomial is an eigenvector of $Ab(G)$. However, sometimes it is not – for example, $Ab(BI)$ is trivial, so all invariants are the eigenvectors, but only the choice of homogeneous ones gives a correct result.

Definition 5.2.3. By $\sigma_i(a,b) \in \mathbb{C}[a,b]^{[G,G]}$ for $i = 1,2,3$ we denote homogeneous polynomials satisfying conditions in Remark 5.2.2, i.e. eigenvectors of the action of $Ab(G)$ on $\mathbb{C}[a,b]^{[G,G]}$ such that the set $\{\sigma_1(a,b), \sigma_2(a,b), \sigma_3(a,b)\}$ generates $\mathbb{C}[a,b]^{[G,G]}$ as a $\mathbb{C}$-algebra.
We will assume that they are ordered such that the numbers $\deg(\sigma_i) \cdot (\alpha_i)_{n_i+1}$ are equal (as usually, α_i denotes the vector of exponents in the i-th monomial in the equation of $\mathrm{Spec}(\mathrm{Cox}(X))$, see Construction 4.1.22).

In the description of ϕ we also use the characters of the Picard torus T, so we recall and introduce some notation.

Notation 5.2.4. As before, $\chi_i(t_0,\ldots,t_{n-1})$ denotes the monomial with exponents given by the i-th column of U, i.e. the i-th character of the Picard torus T used to define its action on $\mathbb{C}^{n+3}$ in Definition 4.1.2. Also, when we write χ_{x_i}, χ_{y_0} or $\chi_{y_{i,j}}$, we think of the character from $\{\chi_1,\ldots,\chi_{n+3}\}$ which corresponds to the respective variable of the coordinate ring A of $\mathbb{C}^{n+3}$ (the order of their appearance is as in the definition of A above).

We start from defining a homomorphism

$$\overline{\phi}\colon A \longrightarrow \mathrm{Cox}(\mathbb{C}^2/G) \otimes \mathbb{C}[T]$$

and then prove that it factors through $\mathrm{Cox}(X) = A/I(S)$, where $I(S)$ is the ideal of $\mathrm{Spec}(\mathrm{Cox}(X))$ in A.

Definition 5.2.5. Define $\overline{\phi}\colon A \longrightarrow \mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1},\ldots,t_{n-1}^{\pm 1}]$ as follows:

$$\begin{aligned}
\overline{\phi}(x_i) &= \sigma_i(a,b)\chi_{x_i}(t_0,\ldots,t_{n-1}),\\
\overline{\phi}(y_0) &= \chi_{y_0}(t_0,\ldots,t_{n-1}),\\
\overline{\phi}(y_{i,j}) &= \chi_{y_{i,j}}(t_0,\ldots,t_{n-1}) \text{ for } i=1,2,3,\ j=1,\ldots,n_i.
\end{aligned}$$

Lemma 5.2.6. *Using the embedding*

$$S = \mathrm{Spec}(\mathrm{Cox}(X)) \subset \mathbb{C}^{n+3} = \mathrm{Spec}(A)$$

given by equation 4.1.3.1 generating the ideal $I(S) \subset A$, the homomorphism $\overline{\phi}$ factors through

$$\phi\colon A/I(S) = \mathrm{Cox}(X) \longrightarrow \mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1}, t_1^{\pm 1}, \dots, t_{n-1}^{\pm 1}].$$

Proof. We show that the image under $\overline{\phi}$ of the equation of $\mathrm{Spec}(\mathrm{Cox}(X))$, described in Construction 4.1.22, is zero. This equation is the sum of three monomials corresponding to branches of the minimal resolution diagram. The vector of exponents of the i-th monomial is α_i, which is orthogonal to the i-th branch (see Definition 4.1.5). This condition translates exactly to the fact that the image of the i-th monomial under $\overline{\phi}$ is $t_0 \cdot \sigma_i(a,b)^{(\alpha_i)_{n_i+1}}$. Hence it is sufficient to show that

$$\sigma_1(a,b)^{(\alpha_1)_{n_1+1}} + \sigma_2(a,b)^{(\alpha_2)_{n_2+1}} + \sigma_3(a,b)^{(\alpha_3)_{n_3+1}} = 0.$$

From Lemma 4.1.17 we know that $(\alpha_i)_{n_i+1} = p_i$, i.e. the numerator of the fraction describing the i-th branch of the resolution diagram. We compare these numbers to the exponents in equations of Du Val singularities $\mathbb{C}^2/[G,G]$, exactly as in the proof of Proposition 4.2.10 – they are the same. Hence it is enough to check that $\sigma_1(a,b), \sigma_2(a,b), \sigma_3(a,b)$ satisfy the single relation in $\mathbb{C}[a,b]^{[G,G]}$ (up to multiplication by some constants). This can be done in a straightforward way, since the sets $\{\sigma_1(a,b), \sigma_2(a,b), \sigma_3(a,b)\}$ for all small subgroups $G \subset GL(2,\mathbb{C})$ are listed in Example 5.3.2. □

Notation 5.2.7. We denote by

$$\psi\colon \mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1}, \dots, t_{n-1}^{\pm 1}] \longrightarrow \mathbb{C}[a,b]^{[G,G]}$$

the homomorphism of evaluation at $t_0 = \ldots = t_{n-1} = 1$, that is $\psi|_{\mathbb{C}[a,b]^{[G,G]}} = id$ and $\psi(t_i) = 1$ for $i = 0, \dots, n-1$. In a geometric picture it is just an embedding of $\mathbb{C}^2/[G,G]$ in $\mathbb{C}^2/[G,G] \times T$ to $\mathbb{C}^2/[G,G] \times \{1\}$.

Note that the composition $\psi \circ \phi$ is the map $\mathrm{Cox}(X) \to \mathrm{Cox}(\mathbb{C}^2/G)$ induced by pushing forward of divisor classes and associated push-forward of sections of corresponding sheaves.

Lemma 5.2.8. *The homomorphism ϕ is a monomorphism.*

Proof. Assume that a polynomial $w \in A$ is in $\ker \overline{\phi}$. Multiplying w by a suitable $v \in A$ which does not contain x_3 and subtracting some multiple of the generator of the ideal $I(S) \subset A$ of $S = \mathrm{Spec}(\mathrm{Cox}(X))$, we get $w' \in \ker \overline{\phi}$ such that its degree as a polynomial of one variable x_3 is smaller than $(\alpha_3)_{n_3+1}$.

Consider $\psi(\overline{\phi}(w'))$, think of it as of an expression in σ_1, σ_2, σ_3 (see Definitions 5.2.3 and 5.2.5). It is 0, so this expression must be divisible by the single relation between σ_1, σ_2, σ_3. But this is impossible, because the degree of this expression as a polynomial of σ_3 is too small. This means that if we look at w' as a polynomial of x_3 again, the polynomials of variables x_1, x_2, y_0, $y_{i,j}$ which are its coefficients are mapped by $\overline{\phi}$ to 0.

However, σ_1, σ_2 and these characters $\chi_i(t_0, \dots, t_{n-1})$ which do not correspond to the variables x_i are independent. To obtain the independence of this set of characters we use the fact that the columns of the matrix U_0 of intersection numbers of components of the exceptional fiber of X are linearly independent. Moreover, σ_1 and σ_2 are independent, because the relation in $\mathbb{C}[a,b]^{[G,G]}$ involves σ_3. Therefore all coefficients of w' viewed as a polynomial of x_3 are just 0, so $wv \in I(S)$ and finally, because $I(S)$ is prime and $v \notin I(S)$, we obtain $w \in I(S)$. □

As a direct result of Lemmata 5.2.6 and 5.2.8 we obtain

Theorem 5.2.9. $\mathrm{Cox}(X) \subset \mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1}, t_1^{\pm 1}, \ldots, t_{n-1}^{\pm 1}]$ *is generated by the images of the variables under* ϕ*, as listed in Definition 5.2.5, i.e.*

1. $\sigma_i(a,b) \cdot \chi_{k(i)}(t_0, \ldots, t_{n-1})$ *for* $i = 1, 2, 3$ *and*

2. $\chi_0(t_0, \ldots, t_{n-1})$ *and* $\chi_{k_{i,j}}(t_0, \ldots, t_{n-1})$ *for* $i = 1, 2, 3,\ j = 1, \ldots, n_i$.

Look at the composition

$$\mathrm{Cox}(X) \xrightarrow{\phi} \mathrm{Cox}(\mathbb{C}^2/G)[t_0^{\pm 1}, t_1^{\pm 1}, \ldots, t_{n-1}^{\pm 1}] \xrightarrow{\psi} \mathrm{Cox}(\mathbb{C}^2/G),$$

that is the push-forward homomorphism between Cox rings. Theorem 5.2.9 mentions two kinds of generators of $\mathrm{Cox}(X)$. These from the first group are pull-backs of generators of $\mathrm{Cox}(\mathbb{C}^2/G)$, which come from the eigenspaces of $Ab(G)$-action on $\mathbb{C}[a,b]^{[G,G]}$. In particular, they are mapped to nontrivial elements of $\mathrm{Cox}(\mathbb{C}^2/G)$ by the push-forward homomorphism. Other are mapped via $\psi \circ \phi$ to $1 \in \mathrm{Cox}(\mathbb{C}^2/G)$, and they depend only on the Picard torus action on $\mathrm{Cox}(X)$, which in fact induces ϕ. We may say that generators of the first kind reflect the structure of the group G and these of the second kind contain the information on the intersection numbers of components in the exceptional divisor of the minimal resolution X. This idea of describing the generators of $\mathrm{Cox}(X)$ seems more general than just the two-dimensional case. In fact, in [DBW13] we prove that for any (minimal) resolution X of a quotient singularity V/G there is a monomorphism

$$\mathrm{Cox}(X) \hookrightarrow \mathrm{Cox}(V/G) \otimes \mathbb{C}[T],$$

constructed using general ideas sketched in this chapter, and we attempt to find generators of this embedding in chosen cases.
The following remark describes a way of thinking of the situation of Theorem 5.2.9, which seems promising, but has not yet been studied thoroughly.

Remark 5.2.10. Define an action of $Ab(G)$ on $\mathbb{C}[a,b]^{[G,G]}[t_0^{\pm 1}, t_1^{\pm 1}, \ldots, t_{n-1}^{\pm 1}]$ as follows: take $g \in G$, then

- the action of g on σ_i is induced from the action on $\mathbb{C}[a,b]$; by definition of σ_i it is multiplication by some $c_i \in \mathbb{C}$,

- the action on the variable $t_{k(i)}$, which is the character of T corresponding to x_i, is multiplication by $1/c_i$ (so that $\phi(x_i)$ are fixed points of this action),

- we require that the remaining characters of T are fixed (with this assumption the action on the coordinates of T is uniquely determined).

Then the image of ϕ is just the invariant ring of this action.

We finish with a few words about the geometric meaning of these results. The dual map to ϕ is just the morphism from the torus bundle to the spectrum of the Cox ring:

$$\phi_{\#}\colon \mathbb{C}^2/[G,G] \times T \longrightarrow \mathrm{Spec}(\mathrm{Cox}(X)).$$

Since ϕ is a monomorphism, the dual $\phi_{\#}$ is a dominant map. And from Remark 5.2.10 it follows that this is the quotient by the action of $Ab(G)$ described therein.

5.3 Examples

The examples below describe the homomorphism ϕ and the generators of $\mathrm{Cox}(X)$ explicitly in a few interesting cases. Also, in Example 5.3.2, we list the eigenvectors of $Ab(G)$ which generate $\mathbb{C}[a,b]^{[G,G]}$ for all small groups $G \subset GL(2,\mathbb{C})$.

Example 5.3.1 (Binary dihedral groups BD_{4n})**.** We consider the case of Du Val singularities, which was investigated in [FGAL11] but without describing generators of the Cox ring. In this example we correct a mistake in [FGAL11, p. 9] – below we provide a set of equations for an embedding of the du Val singularity D_n for odd n in $\mathbb{C}^6$.
The commutator subgroup of BD_{4n} is $\mathbb{Z}_n = \langle \mathrm{diag}(\varepsilon_n, \varepsilon_n^{-1})\rangle$. The ring of invariants of the action of $[BD_{4n}, BD_{4n}]$ on $\mathbb{C}[x,y]$ is generated by xy, x^n and y^n. However, only the first monomial is an eigenvector of the action of $Ab(BD_{4n})$ on this ring of invariants and we have to find suitable linear combinations of the remaining two (see Example 5.3.2). As before, the coordinates on $\mathbb{C}^2 \times (\mathbb{C}^*)^n$ are $(a, b, t_0, \ldots, t_{n-1})$. If n is even then the generators of $\mathrm{Cox}(X)$ are

$$\begin{aligned} \phi(x_j) &: \quad i(a^n + b^n)t_1, (a^n - b^n)t_2, 2^{\frac{2}{n}}abt_{n-1}, \\ \phi(y_0), \phi(y_{i,j}) &: \quad \frac{t_1t_2t_3}{t_0^2}, \frac{t_0}{t_1^2}, \frac{t_0}{t_2^2}, \frac{t_0t_4}{t_3^2}, \frac{t_3t_5}{t_4^2}, \frac{t_4t_6}{t_5^2}, \ldots, \frac{t_it_{i+2}}{t_{i+1}^2}, \ldots, \frac{t_{n-3}t_{n-1}}{t_{n-2}^2}, \frac{t_{n-2}}{t_{n-1}^2}. \end{aligned}$$

And if n is odd, we have

$$\begin{aligned} \phi(x_j) &: \quad (-ia^n + b^n)t_1, (a^n - ib^n)t_2, 2^{\frac{2}{n}}abt_{n-1}, \\ \phi(y_0), \phi(y_{i,j}) &: \quad \frac{t_1t_2t_3}{t_0^2}, \frac{t_0}{t_1^2}, \frac{t_0}{t_2^2}, \frac{t_0t_4}{t_3^2}, \frac{t_3t_5}{t_4^2}, \frac{t_4t_6}{t_5^2}, \ldots, \frac{t_it_{i+2}}{t_{i+1}^2}, \ldots, \frac{t_{n-3}t_{n-1}}{t_{n-2}^2}, \frac{t_{n-2}}{t_{n-1}^2}. \end{aligned}$$

We can use the formula for ϕ (more precisely, for the associated morphism of varieties) in the case of odd n to correct a false statement on page 9 of [FGAL11]. The authors describe the quotient of $\mathbb{C}^{n+3}$ by the Picard torus action as

$$\begin{aligned} V = \{Z_2^4 - Z_5Z_6 = Z_1Z_2^2 - Z_3Z_4 = Z_2^2Z_4 - Z_3Z_6 = \\ = Z_2^2Z_3 - Z_4Z_5 = Z_4^2 - Z_1Z_6 = Z_3^2 - Z_1Z_5 = 0\} \end{aligned}$$

and attempt to realize $\mathbb{C}^2/BD_{4n}$ as a subvariety of V. They suggest that it is isomorphic to

$$V' = V \cap \{Z_1^k + Z_3 + Z_4 = 0\},$$

where $k = (n-1)/2$. However, this variety is reducible. One component (of dimension 2) is given by $Z_1 = Z_3 = Z_4 = Z_2^4 - Z_5Z_6 = 0$ and the second one, isomorphic to $\mathbb{C}^2/BD_{4n}$, is the closure of the set of points of V' with at least one of Z_1, Z_3, Z_4 nonzero.

To obtain the full set of equations of the second component we first apply the quotient morphism described in [FGAL11, Lemma 4.2] to the image of ϕ, i.e. we compute monomials $Z_1, \ldots, Z_6$.

The relations between these monomials for a few small values of n can be computed for example in Singular, [DGPS12]. Thus we find two more equations, namely

$$Z_1^{k-1}Z_3 + Z_2^2 + Z_5 = 0 \quad \text{and} \quad Z_1^{k-1}Z_4 + Z_2^2 + Z_6 = 0.$$

It turns out that they are sufficient for all odd n. i.e.

$$V \cap \{Z_1^k + Z_3 + Z_4 = Z_1^{k-1}Z_3 + Z_2^2 + Z_5 = Z_1^{k-1}Z_4 + Z_2^2 + Z_6 = 0\}$$

is irreducible and by a direct computation one can check that its coordinate ring is isomorphic to the one of $\mathbb{C}^2/BD_{4n}$.

This observation does not change anything in the main results of [FGAL11]. However, this is a convincing example that the ideas used there may be hard to generalize to more complicated singularities.

Example 5.3.2. Let G be a finite nonabelian small subgroup of $GL(2,\mathbb{C})$. We compute the eigenvectors of the induced action of $Ab(G)$ which generate $\mathbb{C}[x,y]^{[G,G]}$. We use the list of generators of rings of $[G,G]$-invariants from [DZ93] and Corollary 3.2.5. The data included in this example, together with the description of the exceptional divisor of the minimal resolution of $\mathbb{C}^2/G$ given in section 3.4, is entirely sufficient to write down ϕ explicitly in all considered cases.

1. For $G = BD_{n,m}$ we have $[G,G] \simeq \mathbb{Z}_n \subset SL(2,\mathbb{C})$. The invariants of $[G,G]$ are generated by

   $$xy, \quad x^n, \quad y^n$$

   with the relation $(xy)^n - x^ny^n = 0$. Invariants that are eigenvectors of $Ab(G)$ are

   $$xy, \quad x^n + y^n, \quad x^n - y^n$$

   for even n and

   $$xy, \quad x^n + iy^n, \quad x^n - iy^n$$

   for odd n.

2. For $G = BT_m$ the commutator subgroup is $[G,G] = BD_2$ and its invariants are generated by

   $$x^2y^2, \quad x^4 + y^4, \quad xy(x^4 - y^4)$$

with the relation $-4(x^2y^2)^3 + (x^2y^2)(x^4+y^4)^2 - (xy(x^4-y^4))^2 = 0$. The last polynomial is an invariant of BT, hence also an invariant of $Ab(BT_m)$. The remaining eigenvectors of $Ab(G)$ are

$$x^4 + y^4 + 2i\sqrt{3}x^2y^2 \quad \text{and} \quad x^4 + y^4 - 2i\sqrt{3}x^2y^2.$$

3. For $G = BO_m$ the invariants of $[G,G] = BT$ are generated by

$$A = \sqrt[4]{108}xy(x^4 - y^4),$$
$$B = -(x^8 + 14x^4y^4 + y^8),$$
$$C = x^{12} - 33x^8y^4 - 33x^4y^8 + y^{12}$$

   with the relation $A^4 + B^3 + C^2 = 0$. Moreover, these generators lie in eigenspaces of $Ab(G)$.

4. Finally, for $G = BI_m$ the invariants of $[G,G] = BI$ are generated by

$$D = \sqrt[5]{1728}xy(x^{10} + 11x^5y^5 - y^{10}),$$
$$E = -(x^{20} + y^{20}) + 228(x^{15}y^5 - x^5y^{15}) - 494x^{10}y^{10},$$
$$F = x^{30} + y^{30} + 522(x^{25}y^5 - x^5y^{25}) - 10005(x^{20}y^{10} + x^{10}y^{20})$$

   with the relation $D^5 + E^3 + F^2 = 0$. As before, these generators lie in eigenspaces of $Ab(G)$.

Example 5.3.3. Let us write down the generators of $\mathrm{Cox}(X)$ in a case of $G = BD_{23,39}$. It was already explored in Examples 3.4.4 and 4.1.25, where the dual graph of the exceptional divisor and the extended intersection matrix are shown. As before, choose the coordinates on $\mathbb{C}^{10}$ to be

$$(y_0, y_{1,1}, x_1, y_{2,1}, x_2, y_{3,1}, y_{3,2}, y_{3,3}, y_{3,4}, x_3).$$

We have $[BD_{23,39}, BD_{23,39}] \simeq \mathbb{Z}_{23} \subset SL(2,\mathbb{C})$ and n is odd, so the generators are

$$\phi(x_1) = (-ia^{23} + b^{23})t_1, \quad \phi(x_2) = (a^{23} - ib^{23})t_2, \quad \phi(x_3) = -i\sqrt[23]{4}abt_6,$$
$$\phi(y_0) = t_1t_2t_3t_0^{-3}, \quad \phi(y_{1,1}) = t_0t_1^{-2}, \quad \phi(y_{2,1}) = t_0t_2^{-2},$$
$$\phi(y_{3,1}) = t_0t_4t_3^{-4}, \quad \phi(y_{3,2}) = t_3t_5t_4^{-2}, \quad \phi(y_{3,3}) = t_4t_6t_5^{-2}, \quad \phi(y_{3,4}) = t_5t_6^{-3}.$$

Example 5.3.4. There is a case where the morphism of varieties $\phi_\#$ induced by ϕ is an embedding of the trivial torus bundle over the singularity $\mathbb{C}^2/BI$ in $\mathrm{Spec}(\mathrm{Cox}(X))$: the Du Val singularity E_8. This is because $[BI, BI] \simeq BI$, so the abelianization is trivial. By Remark 5.2.10, the morphism

$$\phi_\#\colon \mathbb{C}^2/[BI,BI] \times (\mathbb{C}^*)^8 \to \mathrm{Spec}(\mathrm{Cox}(X))$$

is then a quotient by the trivial group action, so the image is isomorphic to $\mathbb{C}^2/BI \times (\mathbb{C}^*)^8 \subset \mathrm{Spec}(\mathrm{Cox}(X))$.

The last example comes from [DBW13], where we investigate the homomorphism $\phi\colon \mathrm{Cox}(X) \hookrightarrow \mathrm{Cox}(V/G) \otimes \mathbb{C}[T]$ for a larger class of quotient singularities V/G and some chosen resolutions. We just give a description of the Cox ring of the investigated resolution, without looking into the proof of the general result. While in previous examples we in fact compared the results of Theorems 4.3.3 and 5.2.9, in the next one we rely only on the approach presented in this chapter, that is on Theorem 5.2.9.

Example 5.3.5. Let $G \simeq S_3$ be the symmetric group acting on $V \simeq \mathbb{C}^4$ with coordinates (x_1, y_1, x_2, y_2) by the direct sum of two copies of the standard representation. Then the generators are

$$\varepsilon = \begin{pmatrix} \varepsilon_3 & 0 & 0 & 0 \\ 0 & \varepsilon_3^{-1} & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \varepsilon_3^{-1} \end{pmatrix} \qquad \text{and} \qquad \tau = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

where ε_3 is the third root of unity. The commutator is $[G, G] \simeq \mathbb{Z}_3$ generated by ε and the abelianization is $Ab(G) \simeq \mathbb{Z}_2$. Thus the ring of invariants $\mathbb{C}[V]^{[G,G]}$ is divided into eigenspaces of the action of $\mathbb{Z}_2$, where the non-trivial element is represented by τ (see Lemma 5.1.2). We give a generating set of this ring divided accordingly.

eigenvalue	generators of degree 2	generators of degree 3
1	$x_1y_1,\ x_2y_2,\ x_1y_2 + x_2y_1$	$x_1^3 + y_1^3,\ x_2^3 + y_2^3,\ x_1^2x_2 + y_1^2y_2,\ x_1x_2^2 + y_1y_2^2$
-1	$x_1y_2 - x_2y_1$	$x_1^3 - y_1^3,\ x_2^3 - y_2^3,\ x_1^2x_2 - y_1^2y_2,\ x_1x_2^2 - y_1y_2^2$

We investigate the symplectic resolution X of V/G. Then $\mathrm{Cox}(X)$ is a subring of $\mathrm{Cox}(V/G) \otimes \mathbb{C}[t^{\pm 1}] \simeq \mathbb{C}[V]^{[G,G]} \otimes \mathbb{C}[t^{\pm 1}] \subset \mathbb{C}[x_1, y_1, x_2, y_2, t, t^{-1}]$ generated by

$$\begin{array}{ll} t^{-2}, & \\ x_1y_1,\ x_2y_2,\ x_1y_2 + x_2y_1, & x_1^3 + y_1^3,\ x_2^3 + y_2^3,\ x_1^2x_2 + y_1^2y_2,\ x_1x_2^2 + y_1y_2^2 \\ t(x_1y_2 - x_2y_1), & t(x_1^3 - y_1^3),\ t(x_2^3 - y_2^3),\ t(x_1^2x_2 - y_1^2y_2),\ t(x_1x_2^2 - y_1y_2^2). \end{array}$$

This description of the Cox ring leads to a construction of considered resolution X: we take $\mathrm{Proj}\,\mathrm{Cox}(X)^+$, where $\mathrm{Cox}(X)^+$ is the graded subring of $\mathrm{Cox}(X)$ consisting of nonnegative pieces with t having weight 1 and all the other variables having weight 0.

Chapter 6

Phylogenetic trees: setup and context

In this chapter we introduce the main objects of our interest in the second part of the thesis: combinatorial structures called phylogenetic trees and algebraic varieties which are their geometric models. The first two sections contain basic definitions and properties. Then we attempt to explain the motivation for investigating phylogenetic trees and for doing it by means of algebraic geometry. Finally, in section 6.4 we present the setting for symmetric models of evolutions, which allow to build phylogenetic trees with an associated finite group action. We present different variants of this construction, which can be found in the literature, and choose the settings which will be most interesting for us in the next two chapters.

6.1 Combinatorics of phylogenetic trees

We recall the setting which was developed in [BW07] and [BDW09].

Definition 6.1.1. A **tree** $\mathcal{T}$ is a connected acyclic graph, whose structure will be described by giving

- a set of edges $\mathcal{E} = \mathcal{E}(\mathcal{T})$,
- a set of vertices $\mathcal{V} = \mathcal{V}(\mathcal{T})$,
- the (unordered) boundary map $\partial : \mathcal{E} \to \mathcal{V}^{\wedge 2}$, where $\mathcal{V}^{\wedge 2}$ denotes the set of unordered pairs of distinct elements in $\mathcal{V}$.

We often distinguish one vertex of $\mathcal{T}$ and call it a **root**.

For an edge $e \in \mathcal{E}$ we write $\partial(e) = \{\partial_1(e), \partial_2(e)\}$, or equivalently $e = \langle \partial_1(e), \partial_2(e) \rangle$. We say that v is a vertex of e, or e contains v (denoted $v \in e$), if $v \in \{\partial_1(e), \partial_2(e)\}$.

Definition 6.1.2. The **degree** (or **valency**) $\deg(v)$ of a vertex v is the number of edges which contain v.

Since $\mathcal{T}$ is connected, each of its vertices has positive degree, unless $\mathcal{T}$ is a trivial tree consisting of a single vertex and no edges. We assume that $\mathcal{T}$ does not have 2-valent vertices, since they are insignificant from the point of view of the presented theory.

Definition 6.1.3. A vertex v is called a **leaf** if $\deg(v) = 1$. Otherwise it is called an **inner vertex** or an **inner node**.

The sets of leaves and inner nodes will be denoted $\mathcal{L}$ and $\mathcal{N}$ respectively; then $\mathcal{V} = \mathcal{L} \cup \mathcal{N}$.

Definition 6.1.4. An edge which contains a leaf is called a **petiole**; an edge which is not a petiole is called an **inner edge**.

Definition 6.1.5. If the valency of each inner vertex of $\mathcal{T}$ is m, then $\mathcal{T}$ is called an m**-valent tree**.

To illustrate these definitions we show four trees (or, more precisely, one specific example and representatives of two infinite families), which play a special role in what follows, especially in chapter 8.

Example 6.1.6. The **snowflake** is a 3-valent tree which has four inner vertices; three of them have two petioles attached each and they are connected by inner edges to the fourth one. A **caterpillar** is a 3-valent tree such that there are exactly two inner nodes to which there are attached two petioles, and any other inner node has exactly one petiole attached. An n-caterpillar is a caterpillar with n inner edges. A **claw tree** (or a **star**) $\mathcal{K}_{1,n}$ is a tree with n edges and exactly one inner node. The claw tree with three leaves is called the **tripod**.

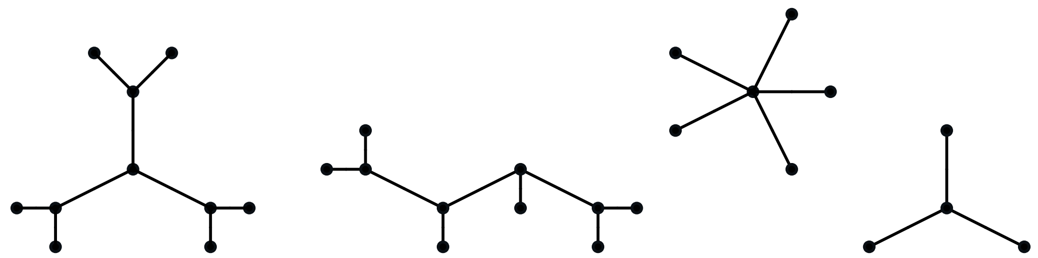


Figure 6.1: The snowflake, the 3-caterpillar, the claw tree $\mathcal{K}_{1,5}$, the tripod $\mathcal{K}_{1,3}$

We now describe the structure of a Markov process on a tree $\mathcal{T}$, again after [BW07] and [BDW09]. Let W be a (complex) vector space of dimension d, which we will call a **model space of states** on the tree $\mathcal{T}$.

Notation 6.1.7. We distinguish a basis of W

$$\mathcal{A} = \{\alpha_1, \alpha_2, \dots \alpha_d\},$$

the elements of which will be called **letters**. We set $\alpha = \alpha_1 + \cdots + \alpha_d$.

Notation 6.1.8. We consider the dual space $W^* = \mathrm{Hom}(W, \mathbb{C})$ with a distinguished basis $\{\alpha_1^*, \dots, \alpha_d^*\}$ dual to $\mathcal{A}$. The pairing of W^* and W will be understood as the action of functionals on vectors, or the other way round, so that

$$\alpha_i(\alpha_j^*) = \alpha_j^*(\alpha_i) = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j. \end{cases}$$

Alternatively, we can think of an inner product chosen on W for which α_i's make an orthonormal basis. Then the product allows to identify W with W^* and α_i with α_i^*.

Definition 6.1.9. A linear map $\sigma : W \to \mathbb{C}$ such that $\sigma(\alpha_i) = 1$ for every i, that is $\sigma = \sum \alpha_i^*$, will be called the **normalization**.

Note that σ is equivalent to α in terms of the above inner product.

Definition 6.1.10. By a **model of evolution** on d letters we understand the pair $(W, \widehat{W})$ (or just the space $\widehat{W}$ if W is fixed), where $\dim W = d$ and $\widehat{W}$ is a subspace of the tensor product $W \otimes W$.

We think of an element $A = \sum_{i,j} a_{ij}(\alpha_i \otimes \alpha_j) \in \widehat{W}$ as of a matrix $A = (a_{ij})$ (by abuse we use the same letter A to denote both), where a_{ij} are obtained by evaluating A on elements of the dual basis, that is $a_{ij} = A(\alpha_i^*, \alpha_j^*)$. Equivalently, the identification $W \simeq W^*$ yields $W \otimes W \simeq W \otimes W^* = \mathrm{End}(W)$ and A can be interpreted as an endomorphism of W.
In addition, we will assume that $\widehat{W}(\sigma, \ \cdot\ ) \subset \mathbb{C} \cdot \alpha$ or, equivalently, that for every matrix $A = \sum_{i,j} a_{ij}(\alpha_i \otimes \alpha_j)$ in $\widehat{W}$ the sum of elements in each row (and, since the matrix is symmetric, also in each column) is the same. This means that, up to multiplication by a constant, elements of $\widehat{W}$ are *doubly stochastic matrices.*
We note that in case when a model of evolution has a group of symmetries which acts transitively on letters (see section 6.4), which is the main case we consider, this assumption turns out to be redundant by Lemma 7.1.1.

Example 6.1.11. Let us show a few natural examples of models of evolution. Remember that in the matrix representation of an element of $\widehat{W}$ the sum of the numbers in each row and each column is the same. If W is of dimension 2 this is equivalent to saying that the matrices in $\widehat{W}$ are of the form

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix}$$

for some a and b in $\mathbb{C}$. Thus $\widehat{W}$ is of dimension 2, and this is the only interesting example for $d = 2$, since any proper subspace of $\widehat{W}$ is of dimension ≤ 1 hence trivial when it comes to normalizing. This model is the binary model, or the **two-state Jukes-Cantor model**, also known as the Cavender-Farris-Neyman model.
In general, the (d-state) **Jukes-Cantor model** is defined by the condition that matrices in $\widehat{W}$ have equal entries on the diagonal and equal entries outside the diagonal.
If $d = 4$, which is a case of particular interest in biology, there are a few nontrivial choices for $\widehat{W}$. The most general case, that is the **general Markov model**, consists of the space of all matrices such that the sum of the numbers in each row and each column is the same. Two commonly used options, connected to applications of this theory, are the **Kimura models**: 2-parameter and 3-parameter model (called for short 2-Kimura and 3-Kimura models) with $\dim \widehat{W}$ being 3 and 4 respectively and matrices in $\widehat{W}$ of the form

$$\begin{bmatrix} a & b & c & c \\ b & a & c & c \\ c & c & a & b \\ c & c & b & a \end{bmatrix} \qquad \begin{bmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{bmatrix}$$

Let us explain how to combine a model of evolution $(W, \widehat{W})$ on d letters and a tree $\mathcal{T}$ to obtain a model of a Markov process on a phylogenetic tree.

Definition 6.1.12. Associate with any vertex $v \in \mathcal{V}(\mathcal{T})$ a copy of W, denoted by W_v. With any edge $e \in \mathcal{E}(\mathcal{T})$ associate a copy of $\widehat{W}$, understood as the subspace in the tensor product $\widehat{W}^e \subset W_{\partial_1(e)} \otimes W_{\partial_2(e)}$. To make it possible we have to choose *one of two variants* of this definition:

(a) take $\mathcal{T}$ to be unrooted and the edges of $\mathcal{T}$ to be unordered, but assume that $\widehat{W}$ consists only of symmetric tensors, or

(b) take a rooted tree $\mathcal{T}$ and choose a direction of each edge of $\mathcal{T}$.

Then elements of $\widehat{W}^e$ will be written as matrices $(a^e_{\alpha_i,\alpha_j}) = (a^e_{i,j})$. A triple $(\mathcal{T}, W, \widehat{W})$ constructed this way is called a **model of a Markov process on a phylogenetic tree**.

Remark 6.1.13. Variant (a) of this definition will be used in chapter 7, and in chapter 8 we adopt variant (b). The choice of direction of edges of $\mathcal{T}$ is most commonly done by directing all edges away from the root.

Remark 6.1.14. By abuse of language, we will frequently call the triple $(\mathcal{T}, W, \widehat{W})$ just a **phylogenetic tree**. As the whole structure $(\mathcal{T}, W, \widehat{W})$, not only the shape of the tree, is the object of our interest, this abbreviation should cause no confusion.

6.2 Geometric picture

To a phylogenetic tree $(\mathcal{T}, W, \widehat{W})$ we assign an algebraic variety. In this section we present its construction, in the same way as we did in [BDW09], and in the next one we discuss its meaning and significance for applications.
The boundary map $\partial : \mathcal{E} \to \mathcal{V}^{\wedge 2}$ from Definition 6.1.1 has its incarnation on the level of tensor products of vector spaces associated with both vertices and edges of the tree $\mathcal{T}$. We define a linear map $\widehat{\Psi}_{W,\widehat{W}}$ of tensor products

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

by setting its dual as follows:

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

where α_v stands for an element of the chosen basis $\mathcal{A} = \{\alpha_1, \dots, \alpha_d\}$ of the space W_v. (Recall that, as in Definition 6.1.12, either the edges of $\mathcal{T}$ are directed or $\widehat{W}$ consists of symmetric tensors.) If the model of evolution is known, we will skip the subscripts in $\widehat{\Psi}_{W,\widehat{W}}$ and write just $\widehat{\Psi}$.
Then we may consider the multi-linear map $\widetilde{\Psi}$ associated with $\widehat{\Psi}$:

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

Definition 6.2.1. The **complete affine model** of the phylogenetic tree (or, more precisely, of the Markov process on the phylogenetic tree) $(\mathcal{T}, W, \widehat{W})$ is the closure of the image of $\widetilde{\Psi}$ in $\bigotimes_{v\in\mathcal{V}} W_v$.

Remark 6.2.2. Take any point in the parameter space

$$\left(A^e = (a^e_{ij})\right)_{e\in\mathcal{E}} \in \prod_{e\in\mathcal{E}} \widehat{W}^e$$

and any function assigning elements of the distinguished basis $\mathcal{A}$ to vertices of $\mathcal{T}$

$$\mathcal{V} \ni v \ \mapsto\ \mu(v) \in \{1, 2, \dots d\}.$$

By definition of $\widetilde{\Psi}$, the respective coordinate of the image of the chosen point under the map $\widetilde{\Psi}$ in the tensor product $\bigotimes_{v\in\mathcal{V}} W_v$ is to be calculated as follows:

$$(\otimes_{v\in\mathcal{V}}\ \ \alpha^*_{\mu(v)}) \left(\widetilde{\Psi}\left(A^e = (a^e_{ij})\right)_{e\in\mathcal{E}}\right) \quad = \quad \prod_{e=\langle u,v\rangle\in\mathcal{E}} a^e_{\mu(u)\mu(v)}.$$

Example 6.2.3. Let us compute $\widetilde{\Psi}$ for the binary model on the tripod, the smallest tree which has an inner vertex (see Fig. 6.1 and Example 6.1.11). Let the inner vertex be called v_0 and the leaves v_1, v_2 and v_3. By e_i we denote the edge joining v_0 and v_i. We consider a basis of $\bigotimes_{v\in\mathcal{V}} W_v$ consisting of simple tensors $\alpha^{v_0}_{c_0} \otimes \alpha^{v_1}_{c_1} \otimes \alpha^{v_2}_{c_2} \otimes \alpha^{v_3}_{c_3}$ corresponding to different choices of one of two letters in each vertex, that is $c_i \in \{1, 2\}$. The coefficient of a point at $\alpha^{v_0}_{c_0} \otimes \alpha^{v_1}_{c_1} \otimes \alpha^{v_2}_{c_2} \otimes \alpha^{v_3}_{c_3}$ will be denoted by $q_{c_0c_1c_2c_3}$. Let $w \in \prod_{e\in\mathcal{E}} \widehat{W}^e$ be a point corresponding to assigning a matrix $\begin{pmatrix} a_i & b_i \\ b_i & a_i \end{pmatrix}$ to e_i. Then $\widetilde{\Psi}(w)$ is given by

$$\begin{aligned}
&q_{1111} = a_1a_2a_3, && q_{1112} = a_1a_2b_3, && q_{1121} = a_1b_2a_3, && q_{1122} = a_1b_2b_3,\\
&q_{1211} = b_1a_2a_3, && q_{1212} = b_1a_2b_3, && q_{1221} = b_1b_2a_3, && q_{1222} = b_1b_2b_3,\\
&q_{2111} = b_1b_2b_3, && q_{2112} = b_1b_2a_3, && q_{2121} = b_1a_2b_3, && q_{2122} = b_1a_2a_3,\\
&q_{2211} = a_1b_2b_3, && q_{2212} = a_1b_2a_3, && q_{2221} = a_1a_2b_3, && q_{2222} = a_1a_2a_3.
\end{aligned}$$

The rational map of projective varieties induced by $\widetilde{\Psi}$ will be denoted by Ψ:

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

Definition 6.2.4. The closure of the image of Ψ is called the **complete projective 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.

However, more than in the complete affine and projective models we are interested in smaller varieties, which are built only from some part of the data contained in $(\mathcal{T}, W, \widehat{W})$. The motivation for this attitude will be discussed in section 6.3.

Given a set of vertices of the tree we can 'hide' them by applying the map $\sigma = \sum_i \alpha_i^*$ to their tensor factors. In what follows we will hide all inner nodes and project to the tensor product of model spaces associated with leaves. That is, we consider the map

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

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

Definition 6.2.5. The **affine model** of a phylogenetic tree (or of a Markov process on a phylogenetic tree) $(\mathcal{T}, W, \widehat{W})$, denoted by $X(\mathcal{T}, W, \widehat{W})$, is an affine subvariety of $W_{\mathcal{L}} = \bigotimes_{v\in\mathcal{L}} W_v$, which is the closure of the image of the composition

$$\widetilde{\Phi} = \Pi_{\mathcal{L}} \circ \widetilde{\Psi} \colon \prod_{e\in\mathcal{E}} \widehat{W}^e \longrightarrow W_{\mathcal{L}} = \bigotimes_{v\in\mathcal{L}} W_v.$$

The **projective model**, denoted by $X_{\mathbb{P}}(\mathcal{T}, W, \widehat{W})$ or just $X_{\mathbb{P}}(\mathcal{T})$ if W and $\widehat{W}$ are fixed, is the underlying projective variety in $\mathbb{P}(W_{\mathcal{L}})$.
If we speak of a feature of both affine and projective models, we frequently use the term **geometric model**.

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

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

It is defined by a special linear subsystem in the complete Segre linear system $|\bigotimes_{e\in\mathcal{E}} p^*_{\mathbb{P}(\widehat{W}^e)} \mathcal{O}_{\mathbb{P}(\widehat{W}^e)}(1)|$, 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.

Remark 6.2.6. The coordinates of $\widetilde{\Phi}$ can be computed as follows: for any function $\mathcal{L} \ni v \mapsto \mu(v) \in \{1, 2, \ldots, d\}$, which describes the distribution of letters on leaves of $\mathcal{T}$, the respective coordinate of the tensor product $\bigotimes_{v\in\mathcal{L}} W_v$ is determined by the formula

$$(\otimes_{v\in\mathcal{L}}\ \ \alpha^*_{\mu(v)}) \left(\widetilde{\Phi}\left(A^e = (a^e_{ij})\right)_{e\in\mathcal{E}}\right) \ = \sum_{\widehat{\mu}} \left(\prod_{e=\langle u,v\rangle\in\mathcal{E}} a^e_{\widehat{\mu}(u)\widehat{\mu}(v)}\right)$$

where the sum is taken over all functions $\widehat{\mu} : \mathcal{V} \longrightarrow \{1, 2, \ldots d\}$ which extend μ.

Example 6.2.7. Let us consider again the binary Jukes-Cantor model on the tripod from Example 6.2.3 and describe $\widetilde{\Phi}$ in this case. We write it in the basis of $W_{\mathcal{L}} = \bigotimes_{v\in\mathcal{L}} W_v$ consisting of $\alpha^{v_1}_{c_1} \otimes \alpha^{v_2}_{c_2} \otimes \alpha^{v_3}_{c_3}$, where v_1, v_2, v_3 are leaves and $c_i \in \{1, 2\}$. The coordinate corresponding to $\alpha^{v_1}_{c_1} \otimes \alpha^{v_2}_{c_2} \otimes \alpha^{v_3}_{c_3}$ is denoted by $q_{c_1c_2c_3}$. Then by

Remark 6.2.6 we have $q_{c_1c_2c_3} = q_{1c_1c_2c_3} + q_{2c_1c_2c_3}$, hence we can write these coefficients using the ones given in Example 6.2.3:

$$q_{111} = a_1a_2a_3 + b_1b_2b_3, \quad q_{112} = a_1a_2b_3 + b_1b_2a_3, \quad q_{121} = a_1b_2a_3 + b_1a_2b_3,$$
$$q_{122} = a_1b_2b_3 + b_1a_2a_3, \quad q_{211} = b_1a_2a_3 + a_1b_2b_3, \quad q_{212} = b_1a_2b_3 + a_1b_2a_3,$$
$$q_{221} = b_1b_2a_3 + a_1a_2b_3, \quad q_{222} = b_1b_2b_3 + a_1a_2a_3.$$

6.3 Motivation

We have introduced the combinatorics and geometry behind the construction of phylogenetic trees. Although it is less important for what follows, it has to be said that the setting introduced above is a case of a construction from statistics: a model of a Markov process on a tree. Hence, before we move to defining group action on phylogenetic trees, we explain the motivation for introducing this setting, coming from biology and statistics, after [BDW09, Sect. 1].

Phylogenetics is a branch of science which aims at reconstructing the history of evolution. It relies heavily on methods of statistics and mathematics, including algebraic geometry. A rough idea is to associate an algebraic variety (affine and projective model as defined above) with a history of evolution (of the genetic code), represented by a Markov process on a tree. The vertices of the tree correspond to species and transition matrices assigned to the edges are interpreted as probability of different mutations of genetic code. Leaves of the tree correspond to living species and inner vertices to extinct ones. The general goal is to understand the (most probable) structure of the phylogenetic tree based on the information of living species, and special points of the variety associated to a Markov process on a tree correspond to possible probability distributions on the DNA states of the living species. For a detailed discussion of the biological context the reader is advised to look in [PS05], and now let us discuss briefly the motivation from statistics, without more biological references.

Roughly speaking, from the point of view of statistics, a Markov process on phylogenetic tree is a collection of random variables ξ_v with values in a set of letters associated with vertices of $\mathcal{T}$, together with a collection of rules for inheritance, that is of conditional (or transition) probability, labeled by edges of $\mathcal{T}$.

In the setting of Section 6.1 the space W is spanned on letters from the set $\mathcal{A}$, the model space of states for variables ξ_v. The statistically meaningful domain in W is the probabilistic simplex described by the following conditions in terms of coordinates (basis dual to $\mathcal{A}$): $\mathrm{Im}(\alpha_i^*) = 0$, for all i (i.e. we consider the real part of the complex vector space W), and $\alpha_i^* \geq 0$, for $i = 1, \ldots, d$, and with normalization $\sigma = 1$. Given $v \in \mathcal{V}$, the dual basis of W_v describes probability distribution of the random variable ξ_v. That is, $P(\xi_v = \alpha_i) \sim \alpha_i^*(w_v)$, where w_v is a vector of W_v (we can call w_v the state of $\mathcal{T}$ at vertex v). Here $\sim$ stands for proportionality and this is the form σ which provides a somewhat more accurate definition $P(\xi_v = \alpha_i) = \alpha_i^*(w_v)/\sigma(w_v)$ which makes sense within the real non-negative orthant of W.

The model of evolution, that is the space $\widehat{W}$, is meant to provide the rules according to which the states are inherited along the edges of $\mathcal{T}$. That is, given $e \in \mathcal{E}$, a tensor (or matrix) $A \in \widehat{W}^e$ has entries

$$a_{ij} = A(\alpha_i^*, \alpha_j^*) \sim P(\xi_{\partial(e)_1} = \alpha_i \mid \xi_{\partial(e)_2} = \alpha_j).$$

Here, again, $\sim$ means that the actual equality makes sense when the entries of A are real and non-negative, and the sum of every row (and column) is 1, i.e. when A is doubly stochastic.
In the case of a Markov process on a tree $\mathcal{T}$ we fix a root $r \in \mathcal{V}$ and this implies an order $<$ on $\mathcal{V} = \mathcal{L} \cup \mathcal{N}$: every edge $e \in \mathcal{E}$ is directed, as noted in Remark 6.1.13, which we denote by $e = \langle u < v \rangle$. Random variables ξ_v determine a Markov process on $\mathcal{T}$ if the value of ξ_v depends only on the value of ξ_u, where u is the node immediately preceding v in terms of the order $<$.
This determines the distribution of variables ξ_v in terms of the initial probability distribution at the root and the relative probability along every edge. That is, for any function $\mathcal{V} \ni v \longrightarrow \mu(v) \in \{1, 2, \ldots d\}$

$$P\left(\bigcap_{v \in \mathcal{V}} (\xi_v = \alpha_{\mu(v)})\right) = P\left(\xi_r = \alpha_{\mu(r)}\right) \cdot \left(\prod_{e = \langle u < v \rangle \in \mathcal{E}} P\left(\xi_v = \alpha_{\mu(v)} \mid \xi_u = \alpha_{\mu(u)}\right)\right).$$

We note that this formula is proportional to the one describing the coordinates of the parametrization of the complete affine model of $\mathcal{T}$, with identifications described above, provided that the initial distribution at the root is uniform, that is $P\left(\xi_r = \alpha_i\right) = 1/d$ for $i = 1, \ldots, d$.
The definition of parametrization is an algebraicised (and, moreover, in case of Definition 6.1.12 (a) also unrooted and isotropic) version of what is commonly considered in the literature, see e.g. [SS03, Sect. 8] or [PS05, Sect. 1.4.4], or [DK09]. In the rooted version we always assume that the distribution at the root is uniform, because this simplifies the notation and leads to the results which have nicer geometric description.

6.4 Symmetric models of evolution

In the next two chapters we consider problems connected to a special kind of models of evolution, namely these which have symmetries, i.e. are invariant with respect to a finite group action. Here we introduce general setting for such models, say which cases will be interesting for us in what follows, and explain their relation to other cases in the literature.

6.4.1 General idea

The setting for symmetric models of evolution, which we use throughout this part of the thesis, was presented before in a joint paper [BDW09].

Notation 6.4.1. Let $G \subseteq S_d$ be a subgroup of group of permutations of d elements, which we will identify with the set of letters $\mathcal{A} = \{\alpha_1, \alpha_2, \dots, \alpha_d\}$. We will sometimes confuse $\mathcal{A}$ with its set of indices $\{1, \dots, d\}$ and use the notation

$$g(\alpha_i) = \alpha_{g(i)}$$

for $g \in G$. We say that the subgroup $G \subseteq S_d$ is transitive if its action on $\mathcal{A}$ is transitive.
We extend the action of S_d on letters to a linear action on the vector space W spanned on $\mathcal{A}$. That is, we consider the natural representation $\rho : S_d \longrightarrow GL(W)$ which yields a representation $\rho_G : G \longrightarrow O(W) \subset GL(W)$, where $O(W)$ is the group of orthogonal transformations preserving the inner product on W in which α_i's form an orthonormal basis. If no confusion is likely, we write just g for both $g \in S_d$ as well as for the matrix $\rho_G(g) \in O(W) \subset GL(W)$. That is, for $w \in W$, we write $\rho_G(g)(w) = g \cdot w$, where on the right hand side w is understood as a column of coefficients of w in basis $\mathcal{A}$.

Remark 6.4.2. Recall that the inner product on W, or the choice of the dual basis in W^*, allows us to identify W with W^*. Note that, for $g \in S_d$, we have $\alpha_i^*(\alpha_{g(j)}) = \alpha_{g^{-1}(i)}^*(\alpha_j)$. That is, the right action of G on W^*, defined as

$$\rho_G^*(g)(u) = u \cdot g^{-1} = u \cdot g^t,$$

makes the identification $W \simeq W^*$ G-equivariant.

It follows that the induced action of G on the product $W \otimes W$ can be described in terms of the adjoint action Ad_G of G on $\mathrm{End}(W)$. That is, if an element of $W \otimes W$ is represented by a matrix $A \in \mathrm{End}(W) = W \otimes W^*$ and $g \in G \subset O(W)$ then we have

$$S^2\rho_G(g)(A) = g \cdot A \cdot g^t = g \cdot A \cdot g^{-1} = Ad_G(g)(A).$$

Observation 6.4.3. In plain words, the whole description above means that the permutation $g \in G \subset S_d$ permutes columns and rows of the matrix A as it does with the elements of the set $\mathcal{A}$. That is, if $A = (a_{ij})$ then $g(A)$'s entry in the i-th row and j-th column is

$$(g(A))_{ij} = a_{g^{-1}(i), g^{-1}(j)}.$$

Notation 6.4.4. By $Fix(G)$ or $Fix(\rho_G)$ we will denote the subspace of fixed points of the action ρ_G. Similarly, by $Fix(\rho_G^*)$ or $Fix(Ad_G)$ we denote the fixed point sets of the respective representations.

Clearly, $Fix(\rho_{S_d})$ contains α and its dual contains σ. In fact we have the following easy observation.

Lemma 6.4.5. *A subgroup $G \subset S_d$ is transitive if and only if $Fix(\rho_G) = \mathbb{C} \cdot \alpha$ or, equivalently, $Fix(\rho_G^*) = \mathbb{C} \cdot \sigma$.*

The following definition describes in a very general way the class of models investigated in the next two chapters.

Definition 6.4.6. A model of evolution $\widehat{W} \subset W \otimes W$ on d letters is called **symmetric** if $\widehat{W} = Fix(\rho_G \otimes \rho_G)$ for some transitive group of symmetries $G \subseteq S_d$.

In view of Observation 6.4.3 the elements of $\widehat{W}$ can be identified with matrices whose entries are invariant with respect to simultaneous permutations of rows and columns by elements of the group G.
The following general observation, which is a direct consequence of the constructions in Definitions 6.2.1 and 6.2.5, describes the influence of the assumptions about group action for geometric models of phylogenetic trees.

Proposition 6.4.7. *Let $(\mathcal{T}, W, \widehat{W})$ be a phylogenetic tree such that $(W, \widehat{W})$ has a group of symmetries $G \subseteq S_d$. Then the parametrization maps Ψ and Φ are G-equivariant. In particular*

$$X_{\mathbb{P}}(\mathcal{T}, W, \widehat{W}) \subset \mathbb{P}\left(\left(\bigotimes_{v \in \mathcal{L}} W_v\right)^G\right) \subset \mathbb{P}\left(\bigotimes_{v \in \mathcal{L}} W_v\right).$$

6.4.2 Different variants

We present special cases of Definition 6.4.6 and we state what is known about corresponding geometric models, especially about their toricness. The notion of models with a group action was developed by several authors, which results in some inconsistency in the naming of the objects under consideration. We try to keep the original names of the classes of models if possible.
First of all, we note that in the literature the assumptions on the group action most often are less general than we adopt here, but in [DK09] there is a very general definition of *equivariant models*, where even the space W_v can change when passing from vertex to vertex.
In chapter 7 we consider symmetric models in full generality of possible group actions, but under the assumption that the phylogenetic tree is isotropic, that is using Definition 6.1.12 (a). In fact, the main point of our interest is the combinatorial question about maximal groups which correspond to certain models of evolution and about hierarchy of such models. We present there the results of [BDW09].

Definition 6.4.8. A model $(W, \widehat{W})$ is called an **isotropic model of evolution** if $\widehat{W}$ is contained in the symmetric product $S^2(W)$. If in addition it satisfies Definition 6.4.6, that is $\widehat{W}$ is the space of fixed points of $S^2\rho_G$ for a transitive action of $G \subseteq S_d$ on letters, then it is called an **isotropic symmetric model of evolution**. Phylogenetic trees $(\mathcal{T}, W, \widehat{W})$ for such models of evolution will be called **isotropic (symmetric) phylogenetic trees**.

The assumption of the isotropy of the model corresponds to the time-reversibility of the Markov process. Such models appear in the literature, see e.g. [PS05, Ch. 17], however, not as frequently as models without this feature.

Remark 6.4.9. In general, geometric models of isotropic symmetric phylogenetic trees does not have to be toric varieties – see an example in [Mic12b, Sect. 5.5]. However, our results presented in Section 7.3 together with the results of [Mic11a] allow us to distinguish a good class of isotropic symmetric phylogenetic trees (represented for instance by the 2-Kimura model) whose geometric models are toric.

In chapter 8 we give up the assumption of isotropy, i.e. we work with symmetric models in the setting of Definition 6.1.12 (b). An example of a class of such phylogenetic trees with very good properties is the class of general group-based models.

Definition 6.4.10. Let W be the regular representation of a finite abelian group G (see Definition 1.3.2). For a **general group-based model** we define the subspace $\widehat{W}$ to be the space $\mathrm{End}(W)^G$ of G-invariant endomorphisms of W.

Remark 6.4.11. Because of its good geometric properties and the fact that it contains a few models very important from the point of view of applications, this class of models has been investigated by a lot of people, see e.g. [ES93, SSE93, PS05, SS05]. The toricness of associated geometric models was observed e.g. in [Hen89, SSE93, SS05].

There is also the class of **group-based models**, where $\widehat{W}$ is constructed from the space of fixed points of the action of $\rho_G \otimes \rho_G$ on $W \otimes W$, where W is the regular representation of an abelian group G, by taking some hyperplane sections given by a *labeling function* on G. In other words, the space of transition matrices is a special subspace of the space of transition matrices for some general group-based model. The details can be found e.g. in [SS05, Sect. 3], but we will not use this setting.
Instead, in chapter 8 we concentrate on other extension of the class of general group-based models, suggested (only in the isotropic setting) in [BDW09] and further developed in [Mic11a, Mic12b]. This is a subclass of the class of group-based models and it contains these group-based models which are the most interesting from the point of view of applications, but it is small enough to include only models with good geometric properties.

Definition 6.4.12. Let G be a finite group with a normal abelian subgroup H. Assume that G acts on the set of letters such that the restriction of this action to H is transitive and effective (i.e. W is the regular representation of H) Take $\widehat{W} = Fix(\rho_G \otimes \rho_G) \subseteq W \otimes W$. Then $(W, \widehat{W})$ is called a G-**model**.

In the literature one can find statements that geometric models associated to group-based models of evolution are toric, see e.g. [SS05, Sect. 2], referring to [ES93]. However, this might be not true in such generality. In [Mic11a, Appendix] there is an example, where the discrete Fourier transform does not produce a monomial parametrization of the geometric model. (This method works in the case of general group-based models, and it was suggested in the papers mentioned above to work for all group-based models.) Roughly speaking, if one chooses a submodel of a general group-based model by taking wrong conditions to determine $\widehat{W}$, then the discrete Fourier transform does not behave well.
But, as it is proven in [Mic11a], the class of G-models is free from this drawback.

Theorem 6.4.13. *[Mic11a, 3.19] Let $\mathcal{T}$ be a trivalent tree and $(W, \widehat{W})$ a G-model. Then the geometric model of the phylogenetic tree $(\mathcal{T}, W, \widehat{W})$ is a toric variety.*

Remark 6.4.14. In the next two chapters, by abuse of language, we will frequently use the term *model* both for a model of evolution $(W, \widehat{W})$ and for a geometric model of a phylogenetic tree $(\mathcal{T}, W, \widehat{W})$, at least in cases where $\mathcal{T}$ does not have to be specified.

Example 6.4.15. From the models listed in Example 6.1.11 two are general group-based models. The 3-Kimura model corresponds to $G \simeq \mathbb{Z}_2 \times \mathbb{Z}_2$. The two-state Jukes-Cantor model comes from the action of $\mathbb{Z}_2$.
However, Jukes-Cantor models with d states for $d > 2$ are not general group-based models any more. The space $\widehat{W}$ consists of fixed points of the action of the full symmetric group S_d. This action does not even satisfy the definition of G-models for $d > 4$, since then there is no normal subgroup $H \subset S_d$ with $|H| = d$.
Also the 2-Kimura model is not a general group-based model, but it is a G-model for $H \simeq \mathbb{Z}_4 \lhd G \simeq D_8$.

Chapter 7

Isotropic models of evolution with symmetries

Throughout the present chapter we consider the class of isotropic symmetric models of evolution in the sense of Definition 6.4.8: $\widehat{W}$ is a subspace of the symmetric product S^2W which is the space of fixed points of $S^2\rho_G$ for some transitive action of $G \subseteq S_d$ on the set of letters.
The results presented below were established in a joint project with W. Buczyńska and J. Wiśniewski, see [BDW09]. They concern mainly algebraic and combinatorial properties of isotropic models. This is because the aim of that paper was to find a sensible class of isotropic phylogenetic trees and make preparations for studying associated geometric models later.
The chapter is organized as follows. We start from introducing a notion of saturated groups, whose conjugacy classes are in bijection with (conjugacy classes of) isotropic symmetric models. We note that geometric models of a tree for conjugate groups are isomorphic. Next, in section 7.2, we examine the case when G is hyperbinary, that is when $G = \mathbb{B}^n := \mathbb{Z}_2^n$, $\mathcal{A} = \mathbb{B}^n$, so that $|\mathcal{A}| = 2^n$ and $\mathcal{A}$ can be identified with G with the regular action on itself. Then we discuss the situation when the group of symmetries of an isotropic model contains an abelian subgroup acting transitively on $\mathcal{A}$. This is the situation when our set-up is close to that of G-models, see Definition 6.4.12. From these results it follows that the hyperbinary model is the only isotropic general group-based model, see Proposition 7.2.9 and Theorem 7.2.10. Finally, in the last section we present the results of computations for low-dimensional cases. Using [GAP12] we computed pairs $(G, \widehat{W_G})$ of saturated groups of permutations and their symmetric models of evolution for $|\mathcal{A}| \leq 9$. This part of the chapter should be treated as a large collection of examples. The aim of producing them was to gain insight into rules and relations in the class of isotropic models with symmetries. It might be advisable to have a look into this section before reading sections 7.2 and 7.3.

7.1 Introductory facts

We start from a few simple lemmas following directly from the definition of a symmetric model of evolution. The global assumption is that the considered models are isotropic, but we note when it is not required. The next two sections are devoted to introducing notions of a saturated permutation group and of a faithful subset of the set of letters. We follow [BDW09, Sect. 2].

7.1.1 Some restrictions on $\widehat{W}$

First of all, note that the assumption that matrices in $\widehat{W}$ are doubly stochastic, up to a multiplicative constant, is redundant for transitive groups of symmetries.

Lemma 7.1.1. *Let $G \subseteq S_d$ be a transitive subgroup. If a matrix $A \in S^2W$ is fixed by $S^2\rho_G$ then the sum of rows (columns) of A is constant.*

Proof. Recall that $\alpha = \alpha_1 + \cdots + \alpha_d$, $\sigma = \alpha_1^* + \cdots + \alpha_d^*$ and to show that the sum of rows of A is constant we are to verify the condition that A evaluated on σ is a multiplicity of α. But for every $g \in G \subset O(W)$ we have $A = g \cdot A \cdot g^{-1}$ hence

$$g\left(A(\sigma)\right) = g \cdot g^{-1} \cdot A \cdot (g(\sigma)) = A(\sigma)$$

where the last equality follows by Lemma 6.4.5. The sum of columns of A is constant just because $A = A^t$. □

Remark 7.1.2. Note that we may apply the proof above to the case of non-isotropic symmetric models, but we obtain a weaker result. Only the sum of rows of A must be constant, the sum of columns does not have to be, so A is proportional to a stochastic matrix, which not necessarily is doubly stochastic.

The transitivity of groups $G \subseteq S_d$ implies some bounds on the dimension of $\widehat{W}_G = Fix(S^2\rho_G)$. Isotropy allows to improve them in the case of odd dimension.

Lemma 7.1.3. *If $G \subseteq S_d$ is transitive then $\dim \widehat{W} \le d$. Moreover, if d is odd then $\dim \widehat{W} \le (d+1)/2$.*

Proof. Let us write a general element $A \in \widehat{W}_G$ as a matrix $A = (a_{ij})$ and note that if an element appears in the first row then, because of transitivity, it has to appear in every row. That is, for $i = 1, \dots, d$ there exists $g_i \in G$ such that $g_i(1) = i$ and, for such g_i and any $j = 1, \dots, d$, it holds

$$a_{1,j} = a_{2,g_2(j)} = \cdots = a_{d,g_d(j)}.$$

Therefore the number of linearly independent coefficients in A can not exceed the length of the row, that is d. This proves the first statement of the lemma.
By the same argument all the coefficients on the diagonal of A are equal. By symmetry of A each coefficient outside the diagonal appears the same number of times above the diagonal as below the diagonal. If some element appears exactly once in

one row, it has to appear exactly once in every row. But in this situation it appears d times in A in total, which is impossible when d is odd. Thus every element outside the diagonal appears at least twice in every row, and at least $2d$ times in total, hence the second part follows. □

The above argument can be extended to the following.

Lemma 7.1.4. *Suppose that $G \subseteq S_d$ is transitive. Let $G_1 = G_{\alpha_1} \subset G$ be the subgroup fixing α_1. Then the dimension of $\widehat{W}_G$ does not exceed the number of orbits of G_{α_1} in the set $\mathcal{A}$.*

Proof. Let $g \in G_{\alpha_1}$. Then $g(\alpha_i) = \alpha_j$ implies $a_{1,i} = a_{1,j}$ in the matrix $A = (a_{i,j}) \in \widehat{W}$. Since the other rows of A are obtained by permuting the entries in the first row we get the conclusion. □

Remark 7.1.5. Lemmas 7.1.3 and 7.1.4 work for non-isotropic models with one exception – the inequality $\dim \widehat{W} \leq (d+1)/2$ fails when we do not assume that $A = A^t$.

Remark 7.1.6. We state one more useful fact on $\dim \widehat{W}$. Assume that the action of G on $\mathcal{A}$ is effective, but not free, i.e. there is $g \in G$ which fixes the i-th letter and does not fix the j-th letter. Then $\dim \widehat{W} < d$, because we have the relation $a_{i,j} = a_{i,g(j)}$ identifying two elements in a row.

The boundary cases with regard to the dimension of $\widehat{W}$ are of particular interest. We discuss the case when $\dim \widehat{W} = \dim W$ in the subsequent section, see Proposition 7.2.9.

7.1.2 Saturated subgroups

Before we begin developing the theory, we give an example of an isotropic model of evolution with symmetries. It shows how the assumption of isotropy works together with the invariancy of transition matrices to determine $\widehat{W}$.

Example 7.1.7. Let $h \in S_d$ be a cyclic permutation of length d, say $h = (1, \ldots, d)$, and let $H = \langle h \rangle$ be the group generated by h. Then for $A = (a_{ij}) \in \widehat{W}$ we have

$$a_{11} = a_{22} = \ldots = a_{dd}, \quad a_{ij} = a_{i+1,j+1} = \ldots = a_{i+d,j+d} = a_{ji} = a_{j+1,i+1} = \ldots a_{j+d,i+d},$$

where all operations on indices are performed modulo d. Thus $\widehat{W}_H$ consists of matrices of the form

$$\begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_2 & a_1 \\ a_1 & a_0 & a_1 & \cdots & a_3 & a_2 \\ a_2 & a_1 & a_0 & \cdots & a_4 & a_3 \\ \cdots & \cdots & \cdots & & \cdots & \cdots \\ a_2 & a_3 & a_4 & \cdots & a_0 & a_1 \\ a_1 & a_2 & a_3 & \cdots & a_1 & a_0 \end{pmatrix}$$

where a_i are arbitrary numbers. It follows that $\dim \widehat{W}_H = (d+1)/2$ if d is odd and $d/2+1$ if d is even.
We note that the matrix above can be written as the following linear combination of matrices

$$a_0 \cdot id + a_1 \cdot \left(h + h^{-1}\right) + a_2 \cdot \left(h^2 + h^{-2}\right) + \cdots$$

with h presented as a permutation matrix.
Every such a matrix is symmetric with respect to its center hence, i.e. it is fixed by an involution ν with cyclic decomposition

$$\nu = (1, d)(2, d-1)(3, d-2)\cdots,$$

which satisfies $h^{-1} = \nu \cdot h \cdot \nu^{-1}$. Thus $\widehat{W}_H$ is fixed not only by the cyclic group H, but also by the dihedral group $D_{2d} = \langle h,\ \nu\rangle$. These observations will be generalized in section 7.3.
The isotropic model of evolution presented above will be called the **dihedral model**.

We see that, unlike for instance the situation of general group-based models, the group from which we start generating an isotropic model does not necessarily turn out to be the biggest subgroup of S_d which fixes it. According to this observation we introduce the following definition.

Definition 7.1.8. A subgroup $G \subseteq S_d$ is called **saturated** if for any group H such that $G \subseteq H \subseteq S_d$ and $Fix(S^2\rho_G) = Fix(S^2\rho_H)$, it follows that $H = G$. In other words, G is saturated if it is the stabilizer of $Fix(S^2\rho_G)$.

We have yet another immediate observation and thus a subsequent definition.

Lemma 7.1.9. *There is an inclusion reversing bijection between transitive saturated subgroups of S_d and isotropic symmetric models of evolution on d letter.*

Definition 7.1.10. If $(W, \widehat{W})$ is an isotropic symmetric model of evolution on d letters then its **group of symmetries** is the unique transitive saturated $G \subseteq S_d$ such that $Fix(S^2\rho_G) = \widehat{W}$.

Since conjugating subgroups of S_d is just renaming its elements we can identify models associated with conjugate subgroups.

Proposition 7.1.11. *Let $\mathcal{T}$ be a tree and let $\widehat{W}_H$, $\widehat{W}_G$ be two models of evolution on d letters with groups of symmetries H and G respectively. The inclusion of groups $H \subseteq G \subseteq S_d$ implies an inclusion of geometric models*

$$X(\mathcal{T}, W, \widehat{W}_G) \subset X(\mathcal{T}, W, \widehat{W}_H).$$

If groups G and H are conjugate in S_d then, after some linear change of coordinates in $\mathbb{P}(W_{\mathcal{L}})$, the models $X(\mathcal{T}, W, \widehat{W}_G)$ and $X(\mathcal{T}, W, \widehat{W}_H)$ are equal.

Thus, in what follows we will look at saturated transitive subgroups of S_d up to conjugation (and classify them in low-dimensional cases).

7.1.3 Minimal models of evolution

Let us consider a subset of letters $\mathcal{B} \subset \mathcal{A}$ which spans a vector subspace $W_{\mathcal{B}} \subset W$. We have a decomposition $W = W_{\mathcal{B}} \oplus W_{\mathcal{B}}^{\perp}$, where $W_{\mathcal{B}}^{\perp}$ is spanned by the complement of $\mathcal{B}$, that is $\mathcal{A} \setminus \mathcal{B}$. We fix the projection $\pi_{\mathcal{B}} : W \longrightarrow W_{\mathcal{B}}$, the kernel of which is $W_{\mathcal{B}}^{\perp}$. This projection extends to $S^2\pi_{\mathcal{B}} : S^2W \longrightarrow S^2W_{\mathcal{B}}$. For $G \subseteq S_d$ take $G_{\mathcal{B}} = \{g \in G : g(W_{\mathcal{B}}) \subset W_{\mathcal{B}}\}$. Elements of $G_{\mathcal{B}}$ define symmetries of $W_{\mathcal{B}}$ with $\widehat{W_{\mathcal{B}}} = Fix(S^2\rho_{G_{\mathcal{B}}})$.

Example 7.1.12. Let $g \in G \subseteq S_d$ be an element whose decomposition into cycles contains a cycle of length r. We may assume that the cycle concerns the first r letters, more precisely that $g = (1, \dots, r) \cdots$. We take $\mathcal{B} = \{\alpha_1, \dots, \alpha_r\}$. In terms of symmetric matrices the projection $S^2\pi_{\mathcal{B}}$ is taking the $r \times r$ upper-left corner from the $d \times d$ matrix $A \in S^2W$. In view of example 7.1.7 this implies constraints on the coefficients of matrices in $\widehat{W}$. Namely, for $A = (a_{i,j}) \in \widehat{W}$ we have the following constraints $a_{1,2} = a_{1,r}$, $a_{1,3} = a_{1,r-1}$, etc.

Definition 7.1.13. In the above situation we say that the subset $\mathcal{B} \subset \mathcal{A}$, or the subspace $W_{\mathcal{B}} \subset W$, is **faithful** if $S^2\pi$ determines an isomorphism of $\widehat{W}$ and $\widehat{W_{\mathcal{B}}}$. We say that the model of evolution $(W, \widehat{W})$ with the group of symmetries G is **minimal** if $\mathcal{A}$ contains no proper faithful subset.

Example 7.1.14. The full symmetric group $G = S_d$ is clearly saturated, its symmetric model of evolution is the d-state Jukes-Cantor model (see Example 6.1.11). Then, for any $d > 1$ any subset of $\{\alpha_1, \dots, \alpha_d\}$ consisting of more than one letter yields a faithful inclusion.

7.2 Hyperbinary model of evolution

Based on [BDW09, Sect. 3] we present some results concerning a generalization of the binary model of evolution (see [BW07]).

Construction 7.2.1. Let us consider hyperbinary groups

$$\mathbb{B}^n = (\mathbb{Z}_2)^n,$$

for which we use additive notation (so its elements are binary sequences of length n). It is well known that any finite group whose elements (except the unit) are of order 2 is isomorphic to some $\mathbb{B}^n$.

We define a representation

$$\rho^n : \mathbb{B}^n \longrightarrow GL(\mathbb{C}^{2^n})$$

by induction with respect to n. For $n = 0$ we set $\rho^0 = 1$. Suppose that ρ^n is defined. Let us decompose $\mathbb{B}^{n+1} = \mathbb{B}^n \oplus \mathbb{Z}_2 \cdot e_{n+1}$ with $\mathbb{B}^n \subset \mathbb{B}^{n+1}$ consisting of these elements whose last coordinate is 0, and $e_{n+1} = (0, \dots, 0, 1)$. For the subset $\mathbb{B}^n \subset \mathbb{B}^{n+1}$ we set $\rho^{n+1}_{|\mathbb{B}^n} = \rho^n \oplus \rho^n$ and in addition

$$\rho^{n+1}(e_{n+1}) = \begin{bmatrix} 0 & I^{2^n} \\ I^{2^n} & 0 \end{bmatrix}$$

where I denotes the identity matrix of the respective dimension.

Before discussing the properties of the hyperbinary representation let us recall the following general property of representations of abelian groups: if an abelian group G acts effectively and transitively on a finite set X, then the action is equivalent to the action of G on itself (see Lemma 1.3.1). The complex representation arising from such an action is the *regular representation* of G. We get an immediate corollary.

Lemma 7.2.2. *Let $\mathcal{A}$ be the standard basis of $W_{\mathbb{B}}^n := \mathbb{C}^{2^n}$. Then $\mathbb{B}^n$ acts effectively and transitively on $\mathcal{A}$ and thus the representation ρ^n is equivalent to the regular representation of $\mathbb{B}^n$.*

We identify, via $\rho^n_{|\mathcal{A}}$, the group $\mathbb{B}^n$ with a subgroup of S_{2^n}; that is, ρ^n is then just the restriction of the natural representation of S_{2^n}. Note that all matrices in $\rho^n(\mathbb{B}^n)$ are symmetric. This is a very special feature of $\mathbb{B}^n$ as it follows from the subsequent observation.

Lemma 7.2.3. *Let W be an arbitrary vector space. All matrices (except identity) in the intersection $S^2(W) \cap O(W)$ are of order 2, hence any finite subgroup of $S^2(W) \cap O(W)$ is hyperbinary.*

Proof. $A^2 = A \cdot A^t = A \cdot A^{-1} = 1$. □

Now we determine the model of evolution corresponding to the hyperbinary representation ρ^n. First we introduce the candidate for $\widehat{W}$ in this model.

Definition 7.2.4. Let $\widehat{W_{\mathbb{B}}^n} \subset S^2(W_{\mathbb{B}}^n)$ be the linear subspace spanned by $\rho^n(\mathbb{B}^n)$.

The following lemma will be generalized in the next section, but for the sake of clarity we present here an explicit argument.

Lemma 7.2.5. *The space $\widehat{W_{\mathbb{B}}^n}$ is equal to $Fix(\mathbb{B}^n)$, it is of dimension 2^n and its intersection with $GL(W_{\mathbb{B}}^n)$ is a Cartan torus in $GL(W_{\mathbb{B}}^n)$.*

Proof. The fact that the space $\widehat{W_{\mathbb{B}}^n}$ is of dimension 2^n follows from Lemma 1.3.3 and the linear independence of characters. Here, however, we note easily by induction on n that the matrices in $\rho^n(\mathbb{B}^n)$ are linearly independent. Indeed, since $\mathbb{B}^{n+1} = \mathbb{B}^n + e_{n+1} \cdot \mathbb{B}^n$ then every linear combination of matrices in $\rho_{n+1}(\mathbb{B}^{n+1})$ can be written as

$$A = \sum_{A_i \in \mathbb{B}^n} a_i \begin{bmatrix} A_i & 0 \\ 0 & A_i \end{bmatrix} + \sum_{B_i \in \mathbb{B}^n} b_i \begin{bmatrix} 0 & B_i \\ B_i & 0 \end{bmatrix}$$

which yields the inductive step.
Next, we note that $\widehat{W_{\mathbb{B}}^n} \subset Fix(\mathbb{B}^n)$. For this we are to check that $g \cdot A \cdot g^{-1} = A$ for every $g \in \rho^n(\mathbb{B}^n)$ and $A \in \widehat{W_{\mathbb{B}}^n}$. But this equality is linear with respect to A, so it is enough to check it on the basis of $\widehat{W_{\mathbb{B}}^n}$. There is a basis consisting of elements of $\rho^n(\mathbb{B}^n)$, for which this is obvious.
By the same argument $\widehat{W_{\mathbb{B}}^n} \cap GL(W_{\mathbb{B}}^n)$ is commutative. Hence it is a complex torus. Its dimension is 2^n, hence it is a Cartan subgroup of $GL(W_{\mathbb{B}}^n)$.

Finally, we prove the equality $Fix(\rho^n(\mathbb{B}^n)) = \widehat{W^n_{\mathbb{B}}}$. One inclusion is already proved, so suppose that $A \in S^2(W^n_{\mathbb{B}})$ is such that $g \cdot A \cdot g^{-1} = A$ for every $g \in \mathbb{B}^n$. We may assume that A is invertible. Thus the subgroup of $GL(W^n_{\mathbb{B}})$ generated by $\rho^n(\mathbb{B}^n)$ and A is abelian and thus contained in a Cartan subgroup of $GL(W^n_{\mathbb{B}})$, which must be $\widehat{W^n_{\mathbb{B}}} \cap GL(W^n_{\mathbb{B}})$. □

Lemma 7.2.6. *The group $\mathbb{B}^n \subset S_{2^n}$ is saturated.*

Proof. Suppose that $h \in S_{2^n}$ preserves $\widehat{W^n_{\mathbb{B}}}$. Then, by definition of $\widehat{W^n_{\mathbb{B}}}$, in particular $h \cdot g \cdot h^{-1} = g$ for every $g \in \mathbb{B}^n \subset S_{2^n}$. Thus subgroup H generated by h and $\mathbb{B}^n$ is abelian. Moreover, H acts freely on the set of letters by Remark 7.1.6. Thus we get $|H| \leq 2^n$, that is $H = \mathbb{B}^n$. □

The following statement summarizes our results.

Proposition 7.2.7. *The pair $(W^n_{\mathbb{B}}, \widehat{W^n_{\mathbb{B}}})$, as defined above, is a symmetric model of evolution with group of symmetries $\mathbb{B}^n$.*

By Lemma 7.1.3 we get a corollary.

Corollary 7.2.8. *The hyperbinary model of evolution is minimal in the sense of Definition 7.1.13.*

Phylogenetic trees with the hyperbinary model of evolution will be called just *hyperbinary phylogentic trees.* In the above situation, if $n = 1$ then such a model is just a binary model and if $n = 2$ then it is a 3-Kimura model, see Example 6.1.11. Note also that in general hiperbinary models are general group-based models (see Definition 6.4.10).
The hyperbinary model of evolution is the unique one which admits the biggest possible dimension, equal to the number of letters (recall Lemma 7.1.3).

Proposition 7.2.9. *Let $(W, \widehat{W})$ be an isotropic model of evolution with group of symmetries G such that $\dim \widehat{W} = \dim W$. Then, up to renumbering elements of $\mathcal{A}$ (i.e. up to conjugation in the group of permutations), this model coincides with the hyperbinary model of evolution.*

Proof. The discussion in Example 7.1.12 implies that if the cyclic decomposition of $g \in G$ contains a cycle of length r, and in addition $r > 2$, then in each row of a matrix in $\widehat{W}$ at least two entries are equal. This means that $\dim \widehat{W} < \dim W$, so in the situation described in the lemma G contains only elements of order 2. The action of G on the set of letters is obviously effective, thus the conclusion follows by Lemma 1.3.1. □

To close this section we state the following theorem, whose proof is based on somewhat more general results, reported in section 7.3.

Theorem 7.2.10. *Hyperbinary groups are the only abelian saturated groups.*

Proof. If G is an abelian saturated group then it satisfies assumptions of Proposition 7.3.2. Hence it contains an element ν of order 2 such that for every $g \in G$ we have $\nu \cdot g \cdot \nu = g^{-1}$. Thus every element of G is of order 2 and G is hyperbinary. □

It follows that the hyperbinary model is the only isotropic general group-based model, in the sense of Definition 6.4.10.

7.3 Abelian groups of symmetries

The present section, describing the results of [BDW09, Sect. 5], concerns the case when the group of symmetries of an isotropic model contains an abelian subgroup acting transitively on the set of letters. Let us begin by recalling trivialities regarding actions of abelian groups. The set $\mathcal{A}$, as usual, consists of d letters. Let H be an abelian group acting effectively and transitively on the set $\mathcal{A}$, which yields the regular representation of H on the vector space W spanned by $\mathcal{A}$. Such a representation $\rho_H : H \longrightarrow GL(W)$ can be diagonalized in terms of characters of H (as described in Lemma 1.3.3).
In this situation, we identify H with a subgroup of $GL(W)$ and argue similarly as in Lemma 7.2.5. Let us consider a linear span

$$W_H = \sum_{h \in H} \mathbb{C} \cdot h \subset \mathrm{End}(W).$$

Then $\dim W_H = d$ (because characters are linearly independent) and H acts by multiplications on W_H as the regular representation. Let us set $T_H := W_H \cap GL(W)$. Then T_H is a connected abelian algebraic subgroup of $GL(W)$ of dimension d, hence a Cartan torus in $GL(W)$. Thus, since H is abelian, W_H is the fixed point set of the adjoint action of H on $\mathrm{End}(W)$. By Lemma 1.3.3, the lattice of (algebraic) characters of T_H, $M_H = \mathrm{Hom}(T_H, \mathbb{C}^*)$, has a distinguished basis consisting of characters of H, that is $\widehat{H} = \mathrm{Hom}(H, \mathbb{C}^*)$.
Now we turn to the situation which is our principal interest – we will work in the following setting.

Notation 7.3.1. Let $(W, \widehat{W})$ be an isotropic symmetric model of evolution on the set $\mathcal{A}$ of d letters with the (saturated) group of symmetries $G \subseteq S_d$. Throughout the present section we assume that there exists an abelian subgroup $H \subseteq G$ which acts effectively and transitively on $\mathcal{A}$.

The following result generalizes our observation from Example 7.1.7. We show that if an abelian group H acts effectively and transitively on the set of letters, then one more permutation fixing the invariants of Ad_H can be produced.

Proposition 7.3.2. *In the situation of Notation 7.3.1 there exists an involution $\nu \in G$, $\nu^2 = id$, such that for every $h \in H$ it holds $\nu \cdot h \cdot \nu = h^{-1}$.*

The proof of the above proposition is divided into some steps. Because of transitivity and effectiveness, elements of H can be identified with letters, so that the action

of H on $\mathcal{A}$ is equivalent to the action of H on itself. From now on we use this identification. Also, we use additive notation for H, as for an abelian group, while for permutations and matrices (the group G and H treated as its subgroup) the multiplicative notation is used.
By classification of finite groups we can write H as a product of cyclic groups, that is $H = \mathbb{Z}_{p_1} \times \ldots \times \mathbb{Z}_{p_k}$ for suitable choice of numbers p_i. We have an inclusion of *sets* $H \subset \mathbb{Z}^k$, coming from the natural inclusion $\mathbb{Z}_{p_i} = \{0, 1, \ldots, p_i - 1\} \subset \mathbb{Z}$. This leads to a linear order on H, which is the restriction of the lexicographical order on $\mathbb{Z}^k$ to H. That is, $h_i = (i_1, \ldots, i_k)$ is the i-th element of H with respect to this order, if

$$i = i_1 \cdot p_2 \cdots p_k + i_2 \cdot p_3 \cdots p_k + \cdots + i_k.$$

Now we can write $H = \{h_0, \ldots, h_{d-1}\}$.
We use the map $\nu : \mathbb{Z}^k \to \mathbb{Z}^k$, defined by

$$\nu((i_1, \ldots, i_k)) = (p_1 - 1 - i_1, \ldots, p_k - 1 - i_k).$$

Note that ν is an involution ($\nu^2 = id$) and it can be restricted to the subset H. The restriction, also denoted by ν, is a permutation of elements of H (hence of $\mathcal{A}$) such that $\nu \cdot h \cdot \nu = h^{-1}$ for every $h \in H$. Indeed, in terms of operations within H we have the following identities

$$\nu((i_1, \ldots, i_k)) = (-i_1 - 1, \ldots, -i_k - 1) = -(i_1, \ldots, i_k) - (1, \ldots, 1)$$

(where h is treated as a permutation of H), from which we get $\nu \cdot h \cdot \nu = h^{-1}$. Similarly, we note that for every $h \in H$ we have $h + \nu(h) = -(1, 1, \ldots, 1)$.
It turns out that the involution ν is compatible with the chosen order on H in the sense of the following lemma. (However, this observation will not be used in what follows.)

Lemma 7.3.3. *The map ν satisfies $\nu(h_i) = h_{d-1-i}$.*

Proof. Let $h_i = (i_1, \ldots, i_k)$. Then, by the definition of the chosen order on H, $i = \sum_{m=1}^{k} i_m \cdot p_{m+1} \cdots p_k$. Let

$$h_j = \nu(h_i) = (p_1 - 1 - i_1, \ldots, p_k - 1 - i_k),$$

then

$$j = (p_1 - 1 - i_1) \cdot p_2 \cdots p_k + (p_2 - 1 - i_2) \cdot p_3 \cdots p_k + \ldots + p_k - 1 - i_k =$$
$$= d - 1 - \sum_{m=1}^{k} i_m \cdot p_{m+1} \cdots p_k = d - 1 - i.$$

□

Now Proposition 7.3.2 follows directly from the next lemma.

Lemma 7.3.4. *Let $H = \{h_0, \ldots, h_{d-1}\}$ be as above, with its regular representation (on the set $\mathcal{A} = H$ with the order defined above) denoted by ρ_H. Let $A = (a_{i,j})$ be a symmetric matrix fixed by the induced action $S^2\rho_H$. Then A is also fixed by the involution ν.*

Proof. To simplify the notation we identify h_i with its index i.
We need to show that for any $i, j \in \{0, \ldots d-1\}$ we have $a_{i,j} = a_{\nu(i),\nu(j)}$. Because A is symmetric, this is equivalent to proving $a_{j,i} = a_{\nu(i),\nu(j)}$. However, we noted that $h_i + \nu(h_i) = h_j + \nu(h_j) = -(1, \ldots, 1)$ and thus we can take $h \in H$ such that

$$h = \nu(h_i) - h_j = \nu(h_j) - h_i$$

(the $\pm$ operations are in H). This implies that $h + h_j = \nu(h_i)$ and $h + h_i = \nu(h_j)$. Hence, in terms of the action of H on itself, $h(j) = \nu(i)$ and $h(i) = \nu(j)$. Thus, because A is fixed by H, we get

$$a_{j,i} = a_{h(j),h(i)} = a_{\nu(i),\nu(j)}.$$

□

The above argument can be reversed.

Lemma 7.3.5. *Let H and ρ_H be as in Lemma 7.3.4. Suppose that a matrix $A = (a_{i,j}) \in \mathrm{End}(W)$ is fixed by Ad_H and $Ad(\nu)$. Then A is symmetric.*

Proof. If A is fixed by H then, as above, $a_{j,i} = a_{\nu(i),\nu(j)}$ and since it is fixed by ν it follows that $a_{\nu(i),\nu(j)} = a_{i,j}$. □

As a result we get the following.

Proposition 7.3.6. *Assume that $(W, \widehat{W})$ is a symmetric model of evolution with G, the saturated group of symmetries, satisfying conditions of Notation 7.3.1. Then any matrix $A \in \mathrm{End}(W)$ fixed by Ad_G is symmetric, i.e. $\widehat{W} = Fix(Ad_G)$.*

Proof. By Lemma 7.3.4 the involution ν is in G, hence by Lemma 7.3.5 in $Fix(Ad_G)$ there are only symmetric matrices. □

Corollary 7.3.7. *It follows that, in the situation of Notation 7.3.1, the space $\widehat{W}$ is the centralizer of G in $\mathrm{End}(W)$ or, more precisely, the closure of the centralizer of $\rho(G)$ in $GL(W) \subset \mathrm{End}(W)$.*

Corollary 7.3.8. *From this result and the proof of toricness of G-models [Mic11a, Thm 3.19] it follows immediately that geometric models associated with isotropic symmetric models of evolution satisfying assumptions in Notation 7.3.1, where in addition H is a normal subgroup of G, are toric varieties.*

7.4 Low dimensional models of evolution

In order to have a nontrivial set of examples we determined all transitive saturated subgroups of S_d for $d = \dim W \leq 9$. The computations were done by simple functions written in GAP (see [GAP12]), which were sufficiently effective up to $d = 9$. The code of our program can be found at `www.mimuw.edu.pl/~marysia/isotrees`. This section contains a brief description of the results of the computations (after [BDW09, Sect.4]). They were a useful source of ideas for the investigation of the case of groups of symmetries with a transitive abelian subgroup, presented in the previous section. Classified models are presented together with respective inclusions (or nesting of models, or Felsenstein's hierarchy), cf. [PS05, Sect. 4.5.1], corresponding to inclusions of groups of symmetries up to conjugation.

7.4.1 Short description of the program

First, let us sketch the main ideas of the algorithm used to determine saturated subgroups of S_d. There are two parts of the algorithm:

- find $\widehat{W}_G = Fix(S^2\rho_G)$ for all $G \subset S_d$,
- for each $G \subset S_d$, decide whether it is maximal subgroup fixing $\widehat{W}_G$.

We consider only representatives of conjugacy classes of subgroups, because models of evolution for conjugate groups are the same up to permutation of letters (see Lemma 7.4.1).

The second part of the algorithm is based on functions provided by GAP. The most important one is `LatticeSubgroups`, which returns the lattice of subgroups of S_d, that is the set of all subgroups and the relation of inclusion on this set (up to conjugacy). We also use `MinimalSupergroupsLattice` which, given the lattice of subgroups, calculates all minimal proper supergroups for each subgroup.

Using these functions we check whether the group G is saturated by comparing $\widehat{W}_G$ to $\widehat{W}_H$ for all minimal proper supergroups H of G. However, the function `LatticeSubgroups` is not effective enough to be used in the cases $d \geq 10$. We think that this step can be done more effectively by more subtle algorithms and low-level programming.

We now turn to the first part of the algorithm, that is, to the question of determining $\widehat{W}_G$ for given $G \subset S_d$. Recall that a matrix $(a_{i,j})$ is a fixed point of $S^2\rho_G$ if and only if for each $g \in G$ we have $a_{i,j} = a_{g(i),g(j)}$, so the task is to find the sets of equal matrix entries. Obviously it suffices to consider only the equalities of entries for g in a generating set of G. For generators we choose the result of the GAP function `SmallGeneratingSet` (it returns a generating set which is not necessarily minimal, but the function is much faster than the function which computes a minimal set of generators). An important (but too technical to describe here) step is to find an appropriate data structure for storing information about equal matrix entries. This algorithm is implemented in the function `ModifySymmetricMatrix` in our program.

Surely, much more effective algorithms for this problem can be found, but this idea gives a solution which is short, easy to implement and sufficient for what we needed.

7.4.2 The results

As stated at the beginning of this section, we identify models of evolution which differ only by a permutation of letters, i.e. models determined by conjugate subgroups of S_d. Therefore, we can reformulate lemma 7.1.9 as follows.

Lemma 7.4.1. *There is an inclusion reversing bijection between conjugacy classes of saturated transitive subgroups of S_d and (isomorphism classes of) isotropic symmetric models of evolution on d letters.*

Example 7.4.2. There are 3 possible forms of the model of evolution with $d = 4$ and dihedral group of symmetries D_8 (that is the 2-Kimura model). They are associated with the three conjugate subgroups of S_4, hence the choice of a cyclic permutation of length 4, cf. example 7.1.7.

$$\begin{bmatrix} a & b & c & b \\ b & a & b & c \\ c & b & a & b \\ b & c & b & a \end{bmatrix} \qquad \begin{bmatrix} a & c & b & b \\ c & a & b & b \\ b & b & a & c \\ b & b & c & a \end{bmatrix} \qquad \begin{bmatrix} a & b & b & c \\ b & a & c & b \\ b & c & a & b \\ c & b & b & a \end{bmatrix}$$

To present the relation between models of evolution described by Lemma 7.4.1, i.e. inclusion of their groups of symmetries up to conjugation, we provide diagrams. For each conjugacy class of saturated groups a generating set of a chosen representative is given. We also find minimal models for all examples in the sense of Definition 7.1.13.
As noted in Example 6.1.11, the only (isotropic symmetric) model of evolution for $d = \dim W = 2$ is the binary one (or the two-state Jukes-Cantor model). Also for $d = 3$ there is no choice: the symmetric group S_3 is the only saturated group and its model is the Jukes-Cantor model (in particular $\dim \widehat{W} = 2$).
The smallest nontrivial example of model hierarchy is in $d = 4$. We tackled this case already in Example 6.1.11.

$$\begin{pmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{pmatrix} \longrightarrow \begin{pmatrix} a & b & c & c \\ b & a & c & c \\ c & c & a & b \\ c & c & b & a \end{pmatrix} \longrightarrow \begin{pmatrix} a & b & b & b \\ b & a & b & b \\ b & b & a & b \\ b & b & b & a \end{pmatrix}$$

Figure 7.1: Hierarchy of models of evolution for $d = 4$

The first of the models in Fig. 7.1 is the hyperbinary model for $n = 2$, or 3-Kimura model, which is minimal. The second one, 2-Kimura model, must be minimal as well, because there are no models of evolution with $d < 4$ and $\dim \widehat{W} = 3$. Generators of chosen representatives are given in the table below, where we also indicate the isomorphism type of the group in question. The last entry in each row indicates whether the model is minimal, and if it is not, then the name of a minimal submodel is provided (J–C stands for the two-state Jukes-Cantor model).

group	**type**	**generators**	**model**
$g4\_1$	$\mathbb{Z}_2 \times \mathbb{Z}_2$	$(1,3)(2,4),\ (1,4)(2,3)$	$\mathbb{B}^2$
$g4\_2$	D_8	$(3,4),\ (1,3)(2,4)$	min
$g4\_3$	S_4	$(1,2,3,4),\ (1,2)$	J–C

Dimensions $d = 5$ and $d = 7$ are not very interesting. In each of these cases there are only two models of evolution, one of them being the Jukes-Cantor model associated with the full symmetric group. The other model of evolution in each case is minimal and it is the dihedral model described in Example 7.1.7.

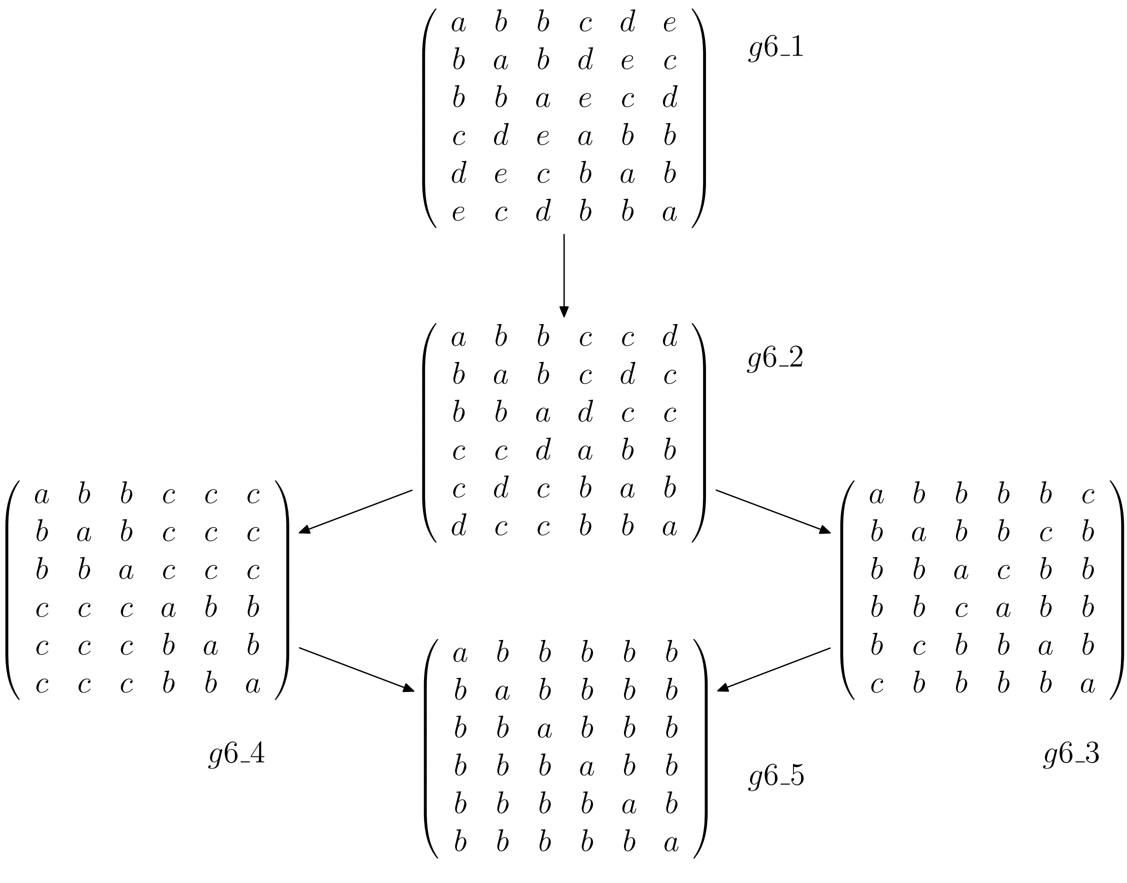


Figure 7.2: Hierarchy of models of evolution for $d = 6$

Fig. 7.2 presents the case of $d = 6$. Only the model of $g6\_1$ is minimal. For the remaining models we can find faithful subspaces of dimension 2, in the case of $g6\_5$, or 4. The set $\{\alpha_2, \alpha_3, \alpha_4, \alpha_5\}$ is faithful in cases of $g6\_2$, $g6\_3$ and $g6\_4$. We give examples of generators of saturated subgroups.

group	**type**	**generators**	**model**
$g6\_1$	D_6	$(1,3,2)(4,5,6),\ (1,6)(2,4)(3,5)$	min
$g6\_2$	D_{12}	$(1,5,3,6,2,4),\ (1,2)(5,6)$	$g4\_1$
$g6\_3$	$\mathbb{Z}_2 \times S_4$	$1,4)(3,6),\ (1,3,6,4),\ (1,5)(2,6)(3,4)$	$g4\_2$
$g6\_4$	$(S_3 \times S_3) \rtimes \mathbb{Z}_2$	$(1,2,3)(5,6),\ (1,5,3,4)(2,6)$	$g4\_2$
$g6\_5$	S_6	$(1,2),\ (1,2,3,4,5,6)$	J–C

In dimension $d = 8$ the relation between models of evolution (see Fig. 7.3) is much more complex than in previous examples (in the subsequent table we skip the description of the isomorphism type of the group in question if it is too long). It can be seen from the following table that only 4 of 11 models of evolution are not minimal. Thus the situation is much different from the cases $d = 6$ (one minimal model) and $d = 9$ (no minimal models).

group	**type**	**generators**	**model**
$g8\_1$	$\mathbb{Z}_2^3$	$(1,2)(3,4)(5,6)(7,8)$, $(1,3)(2,4)(5,7)(6,8)$, $(1,5)(2,6)(3,7)(4,8)$	$\mathbb{B}^3$
$g8\_2$	D_8	$(1,4)(2,3)(5,8)(6,7)$, $(1,7,2,8)(3,6,4,5)$	min
$g8\_3$	$\mathbb{Z}_2 \times D_8$	$(5,6)(7,8),\ (1,3)(2,4)(5,7)(6,8)$, $(1,5)(2,6)(3,7)(4,8)$	min
$g8\_4$	D_{16}	$(1,2)(5,7)(6,8),\ (1,8)(2,5)(3,7)(4,6)$	min
$g8\_5$	$\mathbb{Z}_2^4 \rtimes \mathbb{Z}_2$	$(1,8,4,5)(2,7,3,6)$, $(1,8,3,6)(2,7,4,5)$, $(1,8)(2,7)(3,6)(4,5)$	min
$g8\_6$	$\mathbb{Z}_2 \times S_4$	$(1,3,4,2)(5,7,8,6)$, $(1,7,2,8)(3,6,4,5)$	$g4\_1$
$g8\_7$	—	$(1,5,2,6)(3,7,4,8)$, $(1,5)(2,6)(3,8,4,7)$, $(1,7)(2,8)(3,5,4,6)$	min
$g8\_8$	$(D_8 \times D_8) \rtimes \mathbb{Z}_2$	$(1,4,2,3)(5,8)(6,7)$, $(1,5)(2,6)(3,7,4,8)$, $(1,8,4,6)(2,7,3,5)$	min
$g8\_9$	—	$(1,2)(3,8,4,7)(5,6)$, $(1,5,8,3)(2,6,7,4)$	$g4\_2$
$g8\_10$	$(S_4 \times S_4) \rtimes \mathbb{Z}_2$	$(1,4,3,2)(5,8)(6,7)$, $(1,7,2,5,3,6)(4,8)$	$g4\_2$
$g8\_11$	S_8	$(1,2),\ (1,2,3,4,5,6,7,8)$	J–C

In case of $d = 9$ there are 6 different models of evolution, presented in Fig. 7.4. It turns out that there are no minimal models of evolution on 9 letters. For all models

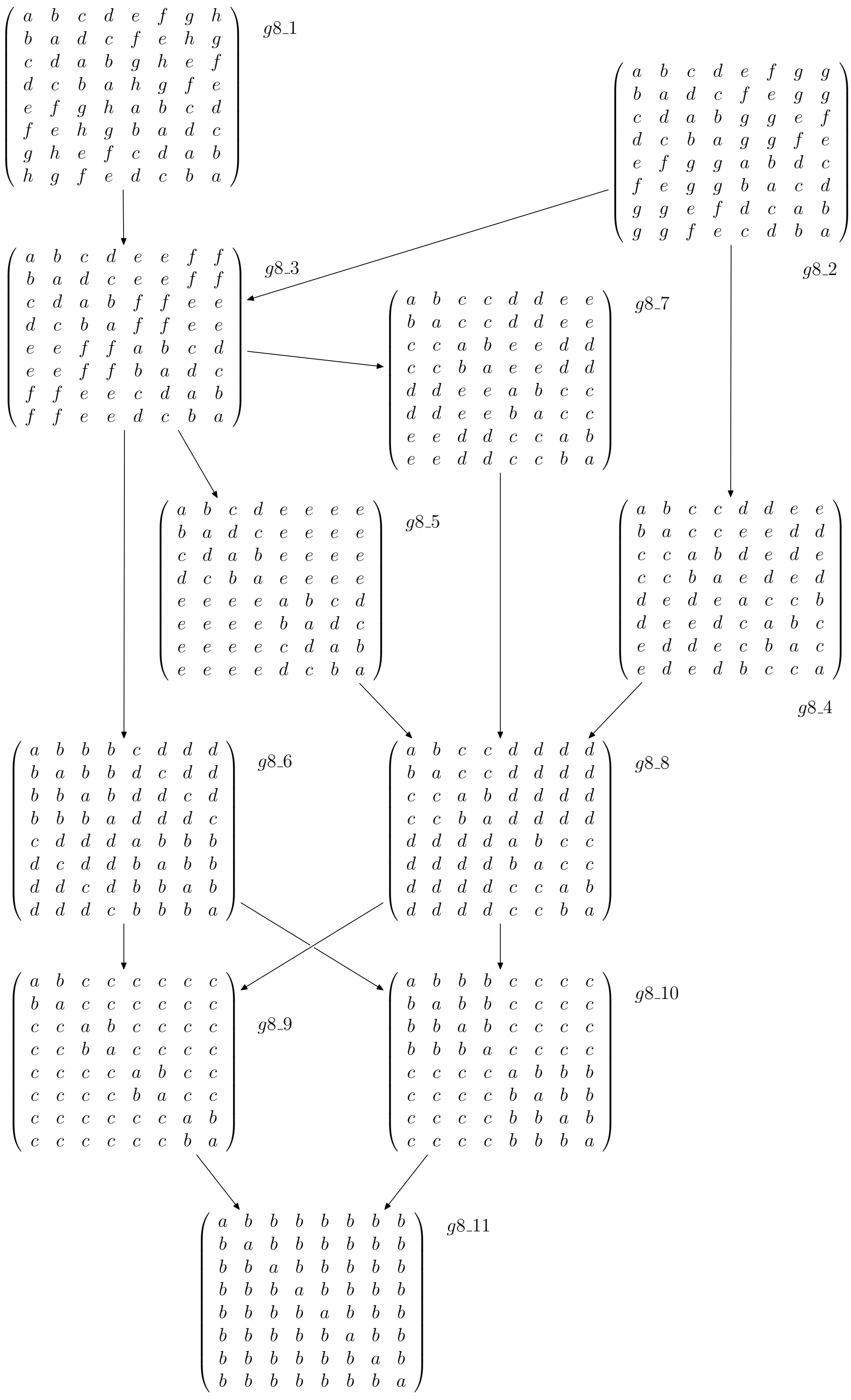


Figure 7.3: Hierarchy of models of evolution for $d = 8$

we can find faithful subspaces of dimension 6, 4 or 2. In all cases a 6-dimensional faithful subspace is spanned by the set of the first 6 basis vectors. For $g9\_3$, $g9\_4$ and $g9\_5$ there also are 4-dimensional faithful subspaces contained in the subspace spanned by the first 6 letters. We give examples of generating sets of saturated groups.

group	**type**	**generators**	**model**
$g9\_1$	$(\mathbb{Z}_3 \times \mathbb{Z}_3) \rtimes \mathbb{Z}_2$	$(2,3)(4,7)(5,9)(6,8)$, $(1,2,3)(4,5,6)(7,8,9)$, $(1,4,7)(2,5,8)(3,6,9)$	$g6\_1$
$g9\_2$	D_{18}	$(1,6)(2,5)(3,4)(7,8)$, $(1,7)(2,9)(3,8)(5,6)$	$g6\_1$
$g9\_3$	$S_3 \times S_3$	$(1,2)(4,5)(7,8)$, $(1,2)(4,8)(5,7)(6,9)$, $(1,8,3,7,2,9)(4,5,6)$	$g4\_1$
$g9\_4$	$(S_3 \times S_3) \rtimes \mathbb{Z}_2$	$(1,5)(3,8)(6,7)$, $(1,7,8,2)(3,4,9,5)$	$g4\_2$
$g9\_5$	—	$(4,5)$, $(1,5,3,4)(2,6)(7,8,9)$, $(1,7,3,9)(2,8)(4,5,6)$	$g4\_2$
$g9\_6$	S_9	$(1,2)$, $(1,2,3,4,5,6,7,8,9)$	J–C

These low-dimensional examples suggest that there are more models of evolution (or classes of saturated subgroups) in even dimensions than in odd dimensions. It is also possible that minimal models appear more often in even dimensions, and most often in dimensions $d = 2^k$. Our examples also yield an observation regarding the family of hyperbinary models: up to dimension 9 there are no other abelian saturated groups. This computational result led us to a general statement in Theorem 7.2.10.

$$\begin{pmatrix} a & b & b & c & d & e & c & e & d \\ b & a & b & e & c & d & d & c & e \\ b & b & a & d & e & c & e & d & c \\ c & e & d & a & b & b & c & d & e \\ d & c & e & b & a & b & e & c & d \\ e & d & c & b & b & a & d & e & c \\ c & d & e & c & e & d & a & b & b \\ e & c & d & d & c & e & b & a & b \\ d & e & c & e & d & c & b & b & a \end{pmatrix} \quad g9\_1$$

$$\begin{pmatrix} a & b & b & c & d & e & e & d & c \\ b & a & b & e & c & d & c & e & d \\ b & b & a & d & e & c & d & c & e \\ c & e & d & a & b & b & c & d & e \\ d & c & e & b & a & b & e & c & d \\ e & d & c & b & b & a & d & e & c \\ e & c & d & c & e & d & a & b & b \\ d & e & c & d & c & e & b & a & b \\ c & d & e & e & d & c & b & b & a \end{pmatrix} \quad g9\_2$$

$$\begin{pmatrix} a & b & b & c & d & d & c & d & d \\ b & a & b & d & c & d & d & c & d \\ b & b & a & d & d & c & d & d & c \\ c & d & d & a & b & b & c & d & d \\ d & c & d & b & a & b & d & c & d \\ d & d & c & b & b & a & d & d & c \\ c & d & d & c & d & d & a & b & b \\ d & c & d & d & c & d & b & a & b \\ d & d & c & d & d & c & b & b & a \end{pmatrix} \quad g9\_3$$

$$\begin{pmatrix} a & b & b & b & c & c & b & c & c \\ b & a & b & c & b & c & c & b & c \\ b & b & a & c & c & b & c & c & b \\ b & c & c & a & b & b & b & c & c \\ c & b & c & b & a & b & c & b & c \\ c & c & b & b & b & a & c & c & b \\ b & c & c & b & c & c & a & b & b \\ c & b & c & c & b & c & b & a & b \\ c & c & b & c & c & b & b & b & a \end{pmatrix} \quad g9\_4$$

$$\begin{pmatrix} a & b & b & c & c & c & c & c & c \\ b & a & b & c & c & c & c & c & c \\ b & b & a & c & c & c & c & c & c \\ c & c & c & a & b & b & c & c & c \\ c & c & c & b & a & b & c & c & c \\ c & c & c & b & b & a & c & c & c \\ c & c & c & c & c & c & a & b & b \\ c & c & c & c & c & c & b & a & b \\ c & c & c & c & c & c & b & b & a \end{pmatrix} \quad g9\_5$$

$$\begin{pmatrix} a & b & b & b & b & b & b & b & b \\ b & a & b & b & b & b & b & b & b \\ b & b & a & b & b & b & b & b & b \\ b & b & b & a & b & b & b & b & b \\ b & b & b & b & a & b & b & b & b \\ b & b & b & b & b & a & b & b & b \\ b & b & b & b & b & b & a & b & b \\ b & b & b & b & b & b & b & a & b \\ b & b & b & b & b & b & b & b & a \end{pmatrix} \quad g9\_6$$

Figure 7.4: Hierarchy of models of evolution for $d = 9$

Chapter 8

Algebraic and geometric properties of symmetric models

The main aim of this chapter is to investigate geometric properties of symmetric models of evolution, mostly general group-based models (see Definition 6.4.10), but a few results concern also a more general class of G-models (see Definition 6.4.12). We concentrate on the case of abelian group of symmetries, since the geometry of corresponding varieties is nontrivial already in this case, and generally they are more important from the point of view of application, however, with some interesting exceptions, like the 2-Kimura model introduced in Example 6.1.11.
We present here the results coming from a joint work with M. Michałek, see [DBM12]. Our project had experimental character and we were looking both for proofs and for counterexamples, so using computer programs for checking small enough cases was an obvious choice. We implemented the algorithm proposed by Michałek in [Mic11a] to determine a combinatorial description (i.e. in terms of toric geometry) of geometric models of chosen phylogenetic trees. In section 8.1, after presenting the set-up for this chapter, we describe this algorithm and the class of models for which it can be used effectively.
In section 8.2 we use our program to investigate normality of geometric models of phylogenetic trees, and section 8.3 is devoted to the problem whether varieties corresponding to a fixed model of evolution, but on different trivalent trees with the same number of leaves, are deformation equivalent. In both cases we get a negative answer. In Proposition 8.2.2 we give examples of non-normal group-based models and in Proposition 8.3.3 we list models for which computing Hilbert-Ehrhart polynomials excluded the possibility of deformation equivalence. This means that [BW07, Thm 3.26] is most probably a phenomenon appearing only in the case of the binary Jukes-Cantor model (the general group-based model with the group of symmetries $G \simeq \mathbb{Z}_2$).
Finally, in section 8.4 we tackle one of the most important problems concerning phylogenetic trees from the point of view of applications, which is computing phylogenetic invariants, i.e. polynomials defining the geometric model. We propose a method of finding ideals of claw trees using a geometric approach, see section 8.4.2. We

conjecture that varieties associated with large claw trees are scheme-theoretic intersections of varieties associated with trees of smaller valency of vertices. This would enable generating the ideals recursively. We prove the conjecture for the Jukes-Cantor model in Proposition 8.4.17. An interesting fact is that we can show that our conjecture is equivalent to the one made by Sturmfels and Sullivant for the 3-Kimura model, see Proposition 8.4.19.

8.1 Toric description of the geometric model

We consider general group-based models in the sense of Definition 6.4.10. By results of [SS05] or [Mic11a, Thm 3.19] their geometric models are toric varieties, not necessarily normal. (In fact, [Mic11a, Thm 3.19] concerns larger class of models, but this property for general group-based model was observed earlier.) These varieties can be described combinatorially by a lattice polytope, see section 2.3. Here we summarize this construction after [Mic11a, Sect. 4] and [DBM12, Sect. 2], writing it finally in a form of an algorithm. Our implementation of this algorithm is a useful tool for computational experiments in problems related to phylogenetics, so in section 8.1.2 we briefly describe the structure and usage of the program.

8.1.1 The polytope of a model

Let $(\mathcal{T}, W, \widehat{W})$ be a phylogenetic tree, as in Definition 6.1.12 (b), i.e. $\mathcal{T}$ is a rooted tree, W denotes a complex vector space of dimension d and $\widehat{W}$ is a subspace of $W \otimes W$. We assume that $(W, \widehat{W})$ is a general group-based model with the (abelian) group of symmetries denoted by G. Thus $d = |G|$ and we can identify a distinguished basis of W with elements of G. Moreover, $\widehat{W}$ is the space of matrices in $W \otimes W$ invariant under Ad_G action, so the phylogenetic tree $(\mathcal{T}, W, \widehat{W})$ is determined by the structure of $\mathcal{T}$ and G. We will use the additive notation for elements of G.

Notation 8.1.1. The phylogenetic tree defined by $\mathcal{T}$ and G as described above will be denoted by $(\mathcal{T}, G)$, the corresponding projective model by $X_{\mathbb{P}}(\mathcal{T}, G)$ and the affine model, which is the affine cone over the projective model, we denote by $X(\mathcal{T}, G)$.

To describe the polytope of $X_{\mathbb{P}}(\mathcal{T}, G)$ we need a definition which generalizes ideas of *networks* and *sockets* introduced in [BW07] for the binary model.

Definition 8.1.2. A **group-based flow** is a function $\mathfrak{n} : \mathcal{E} \to G$, i.e. an assignment of group elements to the edges of $\mathcal{T}$, such that for any inner vertex $v \in \mathcal{V}$, the edge e_0 incoming to v and outgoing edges $e_1, \ldots, e_k$ we have

$$\mathfrak{n}(e_0) = \mathfrak{n}(e_1) + \cdots + \mathfrak{n}(e_k).$$

(For the root we require that the sum of elements assigned to all outgoing edges is zero.) A **socket** is an assignment $\mathfrak{s} : \mathcal{L} \to G$ of group elements to the leaves such that the sum $\sum_{v \in \mathcal{L}} \mathfrak{s}(v)$ is zero (the unit of the group).

It is worth noting that the name *group-based flow* is fully justified. The standard flow condition says that the amount of a fluid incoming to the junction is the equal to the amount of outgoing fluid. Here we may imagine a fluid going through the edges of the tree starting from the root and ending in the leaves, where capacities of edges are the numbers assigned to them. Above we use the reformulation of this condition in terms of the group law. Since all considered flows will be group-based, we often call them just *flows*.

Example 8.1.3. Consider the group $G = \mathbb{Z}_3 = \{0, 1, 2\}$ and the tree in Fig. 8.1.

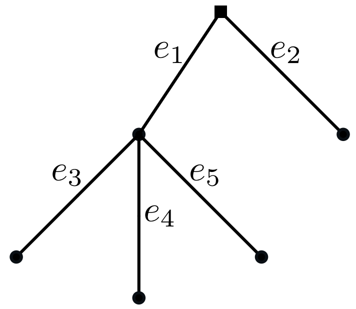


Figure 8.1: A rooted tree with the root marked with a square

Here e_2, e_3, e_4 and e_5 are petioles. By v_i for $i = 2, 3, 4, 5$ we denote the leaf of e_i. An example of a socket is an association $v_2 \to 1$, $v_3 \to 1$, $v_4 \to 2$, $v5 \to 2$.
We can produce a flow from this socket like that: with e_i we associate the same element as with its leaf v_i and moreover $\mathfrak{n}(e_1) := 2$.

Observation 8.1.4. The idea from the example can be generalized to any socket on any tree: we build an assignment starting from petioles and on the higher edges the value of $\mathfrak{n}$ is uniquely determined. Since we start from a socket, the sum of capacities of edges outgoing from the root is indeed 0.
This procedure can be reversed: by assigning to a leaf a value of a flow $\mathfrak{n}$ on its petiole we obtain a socket.

Now we can give the combinatorial description of the polytope of $X_{\mathbb{P}}(\mathcal{T}, G)$. In [Mic11a, Sect.4] an analogous result is proven for all G-models, but this more general version requires additional notation, which will not be used in what follows, hence we restrict to the case of general group-based models. This theorem is based on earlier ideas of [SS05] concerning the toricness of general group-based models.

Theorem 8.1.5 ([Mic11a])**.** *The lattice polytope P_G such that $X_{\mathbb{P}}(\mathcal{T}, G)$ is the projective toric variety X_{P_G} is determined by following conditions:*

- *its vertices lie in a lattice $\widehat{M}$ with basis indexed by pairs (e, g) where e is an edge of a tree and g a group element,*
- *its vertices are in bijection with G-flows on $\mathcal{T}$,*
- *the vertex of P_G associated with a flow n is a sum of all basis elements indexed by such pairs (e, g) that satisfy $\mathfrak{n}(e) = g$.*

We consider the polytope P_G in the sublattice $M \subset \widehat{M}$ spanned by vertices of P_G, i.e. M is the monomial lattice of the toric variety X_{P_G}. Then the only lattice points, that is points of M, in P_G are its vertices.

In this case we can also describe easily the affine model $X(\mathcal{T}, G)$, that is the affine cone over $X_{\mathbb{P}}(T, G)$. By Definition 2.3.2 and Remark 2.3.7, it is a spectrum of the semigroup algebra with a semigroup generated by the lattice points of the polytope P_G.

Remark 8.1.6. Note that different choices of the root of the tree $\mathcal{T}$ give isomorphic polytopes. The corresponding isomorphism of lattices can be written easily in the case when the new root is adjacent to the old one (the group element assigned to the edge joining them is changed to its negative in every flow). By such steps a root can be moved to any position on the tree. Hence we may consider the polytope P_G (and geometric models of $(\mathcal{T}, G)$) without mentioning placement of the root of $\mathcal{T}$. Obviously P_G depends on the choice of the tree $\mathcal{T}$, but since the choice of the tree will always be clear, this information is not contained in the notation for the polytope.

Remark 8.1.7. A useful construction of gluing trees $\mathcal{T}_1$ and $\mathcal{T}_2$ along petioles (that is, one petiole of $\mathcal{T}_1$ is identified with a petiole of $\mathcal{T}_2$, as in Fig. 8.2) has its counterpart in the class of lattice polytopes. The polytope corresponding to obtained tree $\mathcal{T}$ and an abelian group G is the fibre product of polytopes corresponding to $(\mathcal{T}_1, G)$ and $(\mathcal{T}_2, G)$ over the set of coordinates corresponding to identified petioles. The proof can be found in [Sul07, BW07, SS05, Mic11a] – there are different versions depending on the class of considered models.

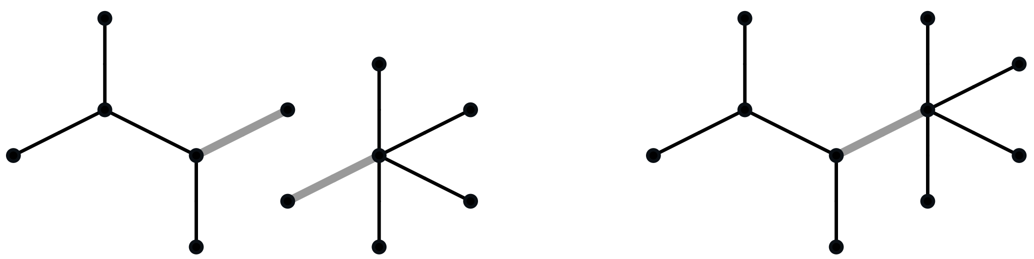


Figure 8.2: Two trees glued along grey petioles

We would like to be able to say something about the ideal of the projective model of a phylogenetic tree, i.e. the ideal of phylogenetic invariants of $(\mathcal{T}, G)$. The observation below follows in a standard way from the description of the polytope P_G, as explained in section 2.3.

Observation 8.1.8. The generating binomials of a toric ideal associated with a polytope P_G correspond to integral relations between lattice points of this polytope (see also Lemma 2.3.3). Hence in our situation the generating set can be created from relations between flows. Such relation can be described in the following way. We number all edges of a tree from 1 to $e = |\mathcal{E}|$. The flows are specific e-tuples of group elements. Each relation of degree m between the flows will be encoded as a pair of matrices with m columns and e rows with group elements as entries. We require that each column represents a flow. Moreover, for $k = 1, \dots, e$ the k-th rows of the matrices should differ by a permutation of entries.

For a general group-based model this is a purely combinatorial description of all phylogenetic invariants for any tree [SS05]. However, it is not a very effective description, since generating sets obtained in this way tend to be large. This construction can be generalized to the class of G-models, see [Mic11a].

Example 8.1.9. Consider the binary Jukes-Cantor model, that is the model corresponding to the group $\mathbb{Z}_2$, and the tree $\mathcal{T}$ in Fig. 8.3.

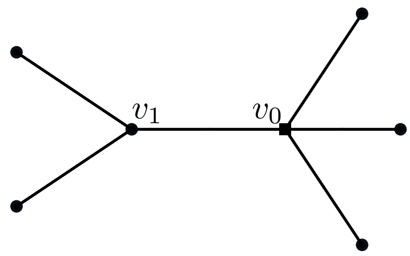


Figure 8.3: A rooted tree with the root v_0 and one inner vertex v_1

We give an example of a relation between lattice points of P_G, hence of a binomial in the ideal of phylogenetic invariants of $(\mathcal{T}, G)$. In vectors containing the information about flows the petioles adjacent to v_1 is represented by first two entries. The third entry corresponds to the inner edge and the last three entries to petioles adjacent to the root v_0. The following pair of matrices denote a relation.

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ \hline 1 & 1 \\ \hline 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ \hline 1 & 1 \\ \hline 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

By definition of a flow (see Definition 8.1.2) the third row has to be both the sum of the first two rows and of the last three rows. Each row of A_1 is indeed a permutation of the corresponding row of A_2.

8.1.2 The algorithm

The first step of all our computations is passing from a phylogenetic tree $(\mathcal{T}, G)$ to the lattice polytope P_G associated with it. The following algorithm, cited after [Mic11a, Sect. 4], written in a form which can be quite easily translated into a computer program, is a direct consequence of Theorem 8.1.5.

Algorithm 8.1.10. The input is the structure of $\mathcal{T}$ and the group law in G. The output, that is the list of vertices of P_G, is computed in the following steps.

1. Choose a root and write all edges of $\mathcal{T}$ as oriented away from the root.

2. For each inner vertex choose one outgoing edge.

3. Fix a bijection b from G to the standard basis of $\mathbb{Z}^{|G|}$.

4. Consider all possible assignments of elements of G to the edges which were not chosen in step 2. There are $|G|^{|E|-|N|}$ such assignments.

5. From each such an assignment make a complete one: to any edge e chosen in step 2 assign $g_e \in G$ to each chosen edge in such a way that the signed sum of elements around each inner vertex gives the unit in G. The signed sum means that we take the negatives of elements assigned to incoming edges. Such completion of an assignment is done top-down, i.e. starting from the root.

6. Each complete assignment gives a vertex of the polytope: $(b(g_e))_{e\in\mathcal{E}}$, where g_e is the element of G associated with edge e.

Our implementation of this algorithm (written in `C++`) can be downloaded from `www.mimuw.edu.pl/~marysia/polytopes` with an instruction and a detailed specification of the input and output data format. It can be used to compute vertices of the polytope associated with a tree given by the user in an input file and one of the groups (with small numbers of elements) defined in the source code. However, extending the program such that it would work for larger class of groups is only a slight modification of a source code.
There are two non-obvious points in the implementation. One is step 2 of the algorithm: making a choice of an outgoing edge from each vertex. It is much easier to choose incoming edge for each vertex except the root and the leaves, as this choice is unique, so we do not need another structure to refer to. Hence what is really done in the program is generating all sockets on $\mathcal{T}$ and completing them to a group flow, as in Observation 8.1.4. Also, if the group operations are precomputed, we indeed obtain the complexity $O(|N||G|^{|E|-|N|})$ predicted in [Mic11a].
As a result we have a fast program which takes a tree in a simple text format as an input and allows to choose one of the groups from the library. It computes the list of vertices of a polytope associated with the input model and outputs it to a text file. It also enables the user to work with this polytope, given as an object of an internal class of the program, in further computations. For example, this simplified significantly the programming necessary to perform the computations of Hilbert-Ehrhart polynomials, described in Section 8.3.

8.2 Normality

Knowing that the projective variety $X_{\mathbb{P}}(\mathcal{T}, G)$ associated with a general group-based model is toric, it is natural to ask whether it is normal. Most theorems in toric geometry work under the assumption of normality. This property can be checked by investigating the corresponding polytope P_G, described in section 2.3. Below we describe our results concerning this question, contained in [DBM12, Sect. 4.1].

Notation 8.2.1. By nP we denote the result of scaling n times a polytope P, called the n-th dilation of P:

$$nP = \{np \colon p \in P\}.$$

We first check whether $X_{\mathbb{P}}(\mathcal{T}, G)$ is projectively normal (see Definition 2.3.4), which corresponds to the condition that for any $n \in \mathbb{N}$ any lattice point in nP_G is a sum of n lattice points of P_G.

Computations described in [Mic11a, Prop. 5.3] have shown that for trivalent trees for the groups $\mathbb{Z}_2$, $\mathbb{Z}_3$, $\mathbb{Z}_4$ and $\mathbb{Z}_2 \times \mathbb{Z}_2$ the associated varieties are projectively normal. However, by [Mic11a, Rem. 5.4], for the 2-Kimura model the associated variety is not projectively normal. Therefore, we wanted to check whether all models for trivalent trees abelian, or maybe at least cyclic, groups are projectively normal. Using our implementation of Algorithm 8.1.10 and Normaliz software (see [BIS]) we were able to check normality for a few more models and these computations gave counterexamples to these questions.

Proposition 8.2.2. *The polytope P_G associated with a phylogenetic tree $(\mathcal{K}_{1,3}, G)$, where $\mathcal{K}_{1,3}$ is the tripod and G is one of the groups $\mathbb{Z}_6$, $\mathbb{Z}_8$, $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$, $\mathbb{Z}_4 \times \mathbb{Z}_2$, is not normal. Hence geometric models $X_{\mathbb{P}}(\mathcal{K}_{1,3}, G)$ are not projectively normal. Moreover, if G is $\mathbb{Z}_5$ or $\mathbb{Z}_7$, then P_G is normal and $X_{\mathbb{P}}(\mathcal{T}, G)$ is projectively normal, hence also normal, for any trivalent tree $\mathcal{T}$.*

Proof. Using our program we can obtain the set of vertices of the polytope related to the investigated group and the tripod. Then we apply Normaliz (see [BIS]) to compute the Hilbert basis of the cone spanned by vertices of P_G. We compare it to the set of vertices of P_G: they are equal if and only if P_G is normal (in the lattice spanned by its vertices). We performed these tests for $\mathbb{Z}_6$, $\mathbb{Z}_8$, $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ and $\mathbb{Z}_4 \times \mathbb{Z}_2$, and in all these cases the result was that the polytope is not normal.

To prove the second statement, we use the fact that the polytope associated with a tree obtained by gluing $\mathcal{T}_1$ and $\mathcal{T}_2$ along petioles is the fibre product of polytopes associated with two trees $\mathcal{T}_1$ and $\mathcal{T}_2$ (see Remark 8.1.7). Moreover, any trivalent tree can be obtained by a series of such identifications, starting from the tripod and adding another tripod to the current tree in each step. Hence, by [Mic11a, Lem. 5.1], if $X_{\mathbb{P}}(\mathcal{K}_{1,3}, G)$ is projectively normal then for any trivalent tree $\mathcal{T}$ the variety $X_{\mathbb{P}}(\mathcal{T}, G)$ is projectively normal. Hence it is sufficient to check whether the polytope P_G associated with the tripod is normal, which we do for $\mathbb{Z}_5$ and $\mathbb{Z}_7$ with the method described above. □

In particular, the class of general group-based models contains models which are not projectively normal. We believe that it may be difficult to characterize the class of groups for which associated geometric models are (projectively) normal, or even to determine an infinite class of (projectively) normal general group-based models. On the other hand there is the following observation.

Lemma 8.2.3. *Let $\mathcal{T}$ be a tree and $G_1 \subset G_2$ be abelian groups. If $X_{\mathbb{P}}(\mathcal{T}, G_1)$ is not projectively normal then $X_{\mathbb{P}}(\mathcal{T}, G_2)$ also is not projectively normal.*

Proof. Let M_i be the lattice with a basis indexed by pairs (e, g), where $e \in \mathcal{E}$ is an edge of $\mathcal{T}$ and $g \in G_i$. The inclusion $G_1 \subseteq G_2$ gives us a natural monomorphism $f \colon M_1 \to M_2$. Let $P_i \subset M_i$ be the polytope associated with the phylogenetic tree $(\mathcal{T}, G_i)$. Note that vertices of P_1 are mapped to vertices of P_2 for G_1-flows on $\mathcal{T}$ are also G_2-flows. Let $\widetilde{M_i} \subset M_i$ be a sublattice spanned by vertices of P_i. Then $f(\widetilde{M_1}) \subset \widetilde{M_2}$.
As P_1 is not projectively normal in the lattice $\widetilde{M_1}$, there exists a point $x \in nP_1 \cap \widetilde{M_1}$ which is not a sum of n vertices of P_1. Let us consider $y = f(x)$. We see that $y \in nP_2 \cap \widetilde{M_2}$. If P_2 was normal in $\widetilde{M_2}$, we would be able to write $y = \sum_{i=1}^{n} q_i$ with $q_i \in P_2$.
Notice that each point in the image $f(M_1)$ has zero on each coordinate corresponding to any (e, g) for $g \in G_2 \setminus G_1$. In particular, y has zeroes on these entries. Since all entries of all vertices of P_2 are nonnegative, this proves that all entries indexed by (e, g) for $g \in G_2 \setminus G_1$ are zero for q_i. However, vertices of P_2 which have all non-zero entries on coordinates corresponding to (e, g) for $g \in G_1$ are in the image of P_1, because they represent G_1-flows on $\mathcal{T}$. Therefore each $q_i = f(p_i)$ for some $p_i \in P_1$. This implies $x = \sum p_i$, hence a contradiction. □

Corollary 8.2.4. *All abelian groups G such that $|G|$ is divisible by 6 or 8 give rise to geometric models of phylogenetic trees which are not projectively normal.*

Let P be the polytope associated with the tripod and the group $\mathbb{Z}_6$. We have already seen that P is not normal, hence the associated affine variety is not normal. However, it is also an interesting question whether the associated projective variety is normal or, equivalently, whether the polytope P is very ample (see Definition 2.3.5; the motivation for this question can be found e.g. in [Bru13]). By direct computation for (any) cone associated with a vertex of the polytope P (see Lemma 2.3.6) we obtain the following result.

Proposition 8.2.5. *Polytope P associated with $(\mathcal{K}_{1,3}, \mathbb{Z}_6)$ is not very ample. Hence the associated projective toric variety is not normal.*

8.3 Deformation equivalence

The question about normality of geometric models of phylogenetic trees is strongly connected to, or even motivated by, deformation problems. It is known that the binary Jukes-Cantor model for trivalent trees has an interesting property: an elementary mutation of a tree gives a deformation of the associated varieties. This implies that binary Jukes-Cantor models of trivalent trees with the same number of leaves are deformation equivalent. The original geometric proof can be found in [BW07] and a new combinatorial one in [Ilt10]. The main result of [Kub10] (obtained before the work presented here was finished) shows that this is not true for the 3-Kimura model. As it was not obvious what to expect for other models, we computed Hilbert functions in a few cases, see [DBM12, Sect. 4.2]. When the geometric model is projectively normal, they are equal to Hilbert-Ehrhart polynomials, see Definition 8.3.1, which are invariants of deformation.

8.3.1 Hilbert-Ehrhart polynomials

We say that two subvarieties $X_1, X_2 \subset \mathbb{P}^m$ are deformation equivalent if their classes are in the same connected component of the Hilbert scheme. In other words, by a well-known theorem of Hartshorne, they are deformation equivalent if and only if they have the same Hilbert polynomial (see [Har66]).

Definition 8.3.1. The Ehrhart polynomial of a lattice polytope P (in lattice M) is the polynomial whose value for $n \in \mathbb{N}$ is the number of lattice points in nP.
The Hilbert function of the projective variety associated with a lattice polytope P maps $n \in \mathbb{N}$ to the number of points with the last coordinate equal to n in the semigroup generated by lattice points of $P \times \{1\}$ in $M \times \mathbb{Z}$. By Remark 2.3.7 and Theorem 8.1.5, in our case this is the same as the number of points in the semigroup generated in M by lattice points (i.e. vertices only) of P such that the sum of first $|G|$ coordinates (corresponding to one edge) is n. Such points will be called *points of degree* n in the semigroup generated by $P \cap M$.
It is known that there exists a polynomial, called the Hilbert polynomial of the projective variety associated with P, such that for n large enough it is equal to the Hilbert function.

Remark 8.3.2. It follows directly from Definition 2.3.5 that the Ehrhart polynomial is equal to the Hilbert function (and then to the Hilbert polynomial), if and only if P is a normal polytope, that is the associated projective variety is projectively normal. We use the term *Hilbert-Ehrhart polynomial* in this case.

The smallest number of leaves which admits at least two different shapes of trivalent trees is six. We investigated geometric models corresponding to the *snowflake* and to the *3-caterpillar* (see Example 6.1.6) and one of a few groups G with $|G| \leq 9$.
By Remark 8.3.2, in cases of normal models we may check the deformation equivalence of geometric models on the snowflake and the 3-caterpillar by computing numbers of lattice points in some multiples of the associated polytopes, called P_G^s and P_G^c respectively. To be precise, the value of the Hilbert-Ehrhart polynomial of $X_{\mathbb{P}}(\mathcal{T}, G)$ in $n \in \mathbb{N}$ is the number of lattice points in nP_G. Hence, even if it is not possible to obtain enough data to determine the whole polynomials (most often because of the memory constraints), in some cases we may decide that Hilbert-Ehrhart polynomials of P_G^s and P_G^c are not equal since their values for some (small) n are different.
The most interesting cases were these of biologically meaningful 2-Kimura and 3-Kimura models. However, before we completed our computations, the numbers of lattice points in $3P_G^s$ and $3P_G^c$ for 3-Kimura model (i.e. $G \simeq \mathbb{Z}_2 \times \mathbb{Z}_2$) were given in [Kub10]. The result implies that varieties associated with these models are not

deformation equivalent. Our computations confirm this result and also give the following.

Proposition 8.3.3. *Varieties associated with 2-Kimura models for the snowflake and the 3-caterpillar trees have different Ehrhart polynomials: there are 56992 lattice points in the second dilation of the corresponding polytope for the snowflake and 57024 for the 3-caterpillar.*
The pairs of geometric models for the snowflake and the 3-caterpillar trees and G being one of $\mathbb{Z}_3$, $\mathbb{Z}_4$, $\mathbb{Z}_5$, $\mathbb{Z}_7$ have different Hilbert-Ehrhart polynomials and therefore are not deformation equivalent.

Proof. Methods used to obtain these results are described in the next section, and precise results of the computations are presented in the Appendix.
For the second statement we use the fact that geometric models for trivalent trees and groups $\mathbb{Z}_3$, $\mathbb{Z}_4$, Z_5, $\mathbb{Z}_7$ are normal, which follows from [Mic11a, Prop. 5.3] and from Proposition 8.2.2 □

Remark 8.3.4. In the cases where G is one of $\mathbb{Z}_8$, $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$, $\mathbb{Z}_9$, the pairs of geometric models for the snowflake and the caterpillar have different Hilbert functions. However, since the models for $\mathbb{Z}_8$ and $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ are not normal and for $\mathbb{Z}_9$ we were not able to check the normality, these results cannot be used to conclude that there is no deformation equivalence in these cases.

8.3.2 A few technical details

Our first attempt to compute numbers of lattice points in consecutive dilations of a polytope was the direct method: constructing the list of lattice points in nP by adding vertices of P to lattice points in $(n-1)P$ and reducing repeated entries. This algorithm is not very efficient, but, after adding a few technical upgrades to the implementation, we were able to confirm the result of [Kub10] concerning the 3-Kimura model. However, this method does not work for non-normal polytopes. Therefore to extend the results and to investigate 2-Kimura model another algorithm had to be implemented.
The second idea was to compute inductively the relative Hilbert polynomials and use the properties of toric fibre product developed in [Sul07] (and used in a slightly different way also by [Kub10] in computations for the 3-Kimura model), described below. This approach involves computing the number of points of degree n in the semigroup generated by lattice points of the polytope, lying in the fibre of the projection onto the set of coordinates $(e, \cdot)$, where e is a fixed petiole and the second parameter runs through G.
We begin with preliminary computations performed for models on the tripod. Let

$$P \subset \mathbb{Z}^{3m} \cong \mathbb{Z}^m \times \mathbb{Z}^m \times \mathbb{Z}^m$$

be the polytope associated with the tripod and a chosen group G, and

$$pr_i : \mathbb{Z}^{3m} \cong \mathbb{Z}^m \times \mathbb{Z}^m \times \mathbb{Z}^m \to \mathbb{Z}^m$$

for $i = 1, 2, 3$ be the projection onto the group of coordinates corresponding to the petiole e_i. Let f_i be a function such that $f_i(a)$ for $a = (a_1, \dots, a_m) \in \mathbb{Z}^m$ is the number of lattice points in $(a_1 + \dots + a_m)P$ that are projected by p_i to a. One of these functions, say $f := f_3$, will be our base for induction. In the program we compute $f(a)$ for sufficiently many values of a to be able to proceed with the algorithm.

Example 8.3.5. The polytope P for the binary Jukes-Cantor model and the tripod has the following vertices:

$$(0,1,0,1,0,1), \quad (0,1,1,0,1,0), \quad (1,0,0,1,1,0), \quad (1,0,1,0,0,1).$$

These are the only lattice points in P, hence in this case $f_i(1,0) = f_i(0,1) = 2$.

Next, we need to compute the number of points of degree n in the fibre of a projection onto two distinguished petioles. Let g_{ij} be the function such that $g_{ij}(a,b)$ for $(a,b) = (a_1, \dots, a_m, b_1, \dots, b_m) \in \mathbb{Z}^m \times \mathbb{Z}^m$ is the number of lattice points of degree $a_1 + \dots + a_m$ that are projected to a by pr_i and to b by pr_j. We choose $g := g_{23}$ and again we compute $g(a,b)$ for sufficiently many pairs (a,b) to proceed with the algorithm.
Let now $\mathcal{T}$ be a tree and P the polytope of $(\mathcal{T}, G)$ with a distinguished petiole e. Let $h_{\mathcal{T}}$ be the function such that $h(a)$ for $a = (a_1, \dots, a_m) \in \mathbb{Z}^m$ is equal to the number of points in the fibre of the projection corresponding to e, of the set of points of degree $a_1 + \dots + a_m$, onto a. We construct a new tree $\mathcal{T}'$ by attaching a tripod to $\mathcal{T}$: a chosen petiole of $\mathcal{K}_{1,3}$ is identified with e as in Remark 8.1.7. Then the polytope associated with $\mathcal{T}'$ is the fibre product of polytopes associated with $\mathcal{T}$ and $\mathcal{K}_{1,3}$. Thus we can calculate the function $h_{\mathcal{T}'}$ for the $\mathcal{T}'$ with the following formula:

$$h_{\mathcal{T}'}(a) = \sum_b g(a,b) h(b),$$

where b runs through the set of all points $b \in \mathbb{Z}^m$ such that $g(a,b) \neq 0$.
This allows us to compute inductively the relative Hilbert function, and the Hilbert function can then be obtained by summing relative ones over all admissible values of a. However, it is better to do the last step in a different way – we perform the last gluing with the tripod and summing in the same time. Suppose that, as before, we are given a tree $\mathcal{T}$ with a distinguished petiole e and a corresponding relative Hilbert function $h_{\mathcal{T}}$. We compute the Hilbert function of the tree $\mathcal{T}'$, which comes from $\mathcal{T}$ by gluing with the tripod along a petiole, using the formula

$$h_{\mathcal{T}'}(n) = \sum_a f(a) h(a),$$

where $a = (a_1, \dots, a_m)$, $\sum a_i = n$, and the function f is our induction base introduced above.
Thus, decomposing the snowflake and the 3-caterpillar (or any other trivalent tree) trees to a sequence of tripods glued along petioles, we can inductively compute (a few small values of) the corresponding Hilbert functions. What is important, using this method one can also compute Ehrhart polynomials for non-normal models,

if only the Ehrhart polynomial for the tripod can be computed. One has only to consider number of lattice points in nP instead of the points of degree n in the semigroup generated by lattice points of P. In particular, for 2-Kimura model some computations turned out to be possible, because its polytope for the tripod is quite well understood (see [Mic11a, Rem. 5.4]) – at least well enough to list lattice points in its second dilation. This way we obtained the results of Proposition 8.3.3.

8.4 Phylogenetic invariants

In this section we investigate the most important objects of phylogenetic algebraic geometry – ideals of phylogenetic invariants, defined as polynomials which give zero for any point of the geometric model of a chosen phylogenetic tree. The main problem is to give an effective description of the whole ideal of phylogenetic invariants of a model, for example in a form of a relatively small generating set.
We present some results concerning this problem in the case of general group-based models. We suggest a way of obtaining all phylogenetic invariants of a general group-based model on a claw tree. More precisely, we conjecture that our method produces invariants which generate the whole ideal of the affine model. If this is true then, together with the results of [SS05], it leads to an algorithm for listing all generators of the ideal of phylogenetic invariants for any general group-based model on any tree. The results of this section were first described in [DBM12, Sect. 3].

8.4.1 Inspirations

The main inspiration for our method are the conjectures stated by Sturmfels and Sullivant in [SS05], recalled below. They are still open but, as we will see in Section 8.4.3, they are strongly connected to the ideas presented in these section. In particular, we prove that our algorithm of obtaining phylogenetic invariants works for trees with more than eight leaves for the 3-Kimura model if we assume that the weaker conjecture of [SS05] holds (see Proposition 8.4.19).
By $\mathcal{K}_{1,n}$ we denote the claw tree with n leaves, as in Example 6.1.11, and G is a finite abelian group. We consider general group-based phylogenetic trees $(\mathcal{K}_{1,n}, G)$.

Definition 8.4.1. By $\phi(G, n) = d$ we denote the least natural number such that the toric ideal of $X(\mathcal{K}_{1,n}, G)$ is generated in degree d. The **phylogenetic complexity** of the group G is defined as

$$\phi(G) = \sup_{n\in\mathbb{N}} \phi(G, n).$$

Based on numerical results Sturmfels and Sullivant suggested in [SS05] the following conjecture.

Conjecture 8.4.2. *[SS05, Conj. 29] For any abelian group G we have $\phi(G) \leq |G|$.*

Because of its importance in applications, the case of the 3-Kimura model was stated as a separate conjecture.

Conjecture 8.4.3. *[SS05, Conj. 30] For* $G \simeq \mathbb{Z}_2 \times \mathbb{Z}_2$ *we have* $\phi(G) \leq 4$*.*

Still very little is known about the function ϕ, apart from the case of the binary Jukes-Cantor model (see also [CP07]):

Proposition 8.4.4. *[SS05, Thm 28] In the case of the binary Jukes-Cantor model* $\phi(\mathbb{Z}_2) = 2$*.*

There are also some computational results supporting these conjectures. To the table in [SS05, Sect. 5] presenting the computations made by Sturmfels and Sullivant a few cases can be added.

Proposition 8.4.5. *We have obtained the following computational results for* $\phi(n, G)$*:*

- $\phi(\mathbb{Z}_3, 6) = 3$,
- $\phi(\mathbb{Z}_5, 4) = 4$,
- $\phi(\mathbb{Z}_8, 3) = 8$,
- $\phi(\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2, 3) = 8$,
- $\phi(\mathbb{Z}_4 \times \mathbb{Z}_2, 3) = 8$.

Proof. After having obtained polytopes for listed models using our implementation of Algorithm 8.1.10, we use `4ti2` software (see [tt]). This program allows to compute the toric ideal for a given semigroup generators. The ideal can be given e.g. in the form of its Markov basis, which is a generating set of a relatively small number of element, but much easier (and quicker) to compute than, for example, the Gröbner basis. Hence we compute Markov bases (which had hundreds of elements in the largest considered cases) and check the degrees of its elements. □

For the 3-Kimura model it is not even known whether the function ϕ is bounded. This question is related to Conjecture 8.4.9 stated in the next section.

8.4.2 A method for obtaining phylogenetic invariants

We propose a method for finding generators of the ideal of phylogenetic invariants, which is not purely algebraic, but inspired by the geometry of considered varieties. First we introduce some notation.

Definition 8.4.6. Let $\mathcal{T}_i$ for $i = 1, 2$ be trees with sets of vertices and edges $\mathcal{V}_i$ and $\mathcal{E}_i$. We say that $\mathcal{T}_1$ is obtained by a **contraction** of an edge e of $\mathcal{T}_2$ if there is a bijection of $\mathcal{V}_1$ with $\mathcal{V}_2'$ equal to $\mathcal{V}_2$ with $\partial_1(e)$ and $\partial_2(e)$ identified, which induces a bijection between $\mathcal{E}_1$ and $\mathcal{E}_2 \setminus \{e\}$. In this situation we say that $\mathcal{T}_2$ is a **prolongation** of $\mathcal{T}_1$.

Example 8.4.7. A tree $\mathcal{K}_{1,6}$ with a root in its inner vertex has two different shapes of prolongations (but if we label vertices, there are more possibilities). The one shown in Fig. 8.4 has two petioles attached to one inner vertex and four to the second one. The other possibility is a tree with three petioles attached to each inner vertex.

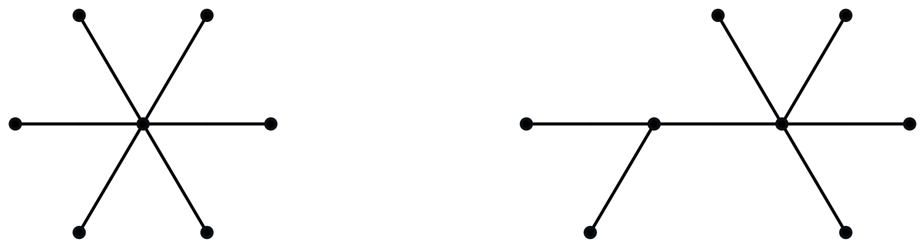


Figure 8.4: $\mathcal{K}_{1,6}$ and one of its prolongations

Remark 8.4.8. Note that these definitions are not the same as the definitions of flattenings introduced in [AR08] and studied in [DK09].

Fix a tree $\mathcal{T}$ and consider the polytope P_G associated with a general group-based model $X(\mathcal{T}, G)$ as in Section 8.1.1. This association is based on the fact that vertices of P_G correspond to G-valued sockets on $\mathcal{T}$. On the other hand, from the toric construction of $X(\mathcal{T}, G)$ we know that vertices of P_G correspond to coordinates of the ambient space of this variety.
Then, if $\mathcal{T}_2$ is a prolongation of $\mathcal{T}_1$ then the variety $X(\mathcal{T}_1, G)$ is in a natural way a subvariety of $X(\mathcal{T}_2, G)$. This is because we have a bijection of sets of leaves $\mathcal{L}_1$ and $\mathcal{L}_2$ of these trees, and the construction of the prolongation allows us to identify sockets on $\mathcal{T}_1$ and $\mathcal{T}_2$. Hence both varieties are contained in $\mathbb{P}^{s-1}$ where s is the number of sockets. The natural inclusion corresponds to the projection of character lattices: in the lattice of $X(\mathcal{T}_2, G)$ we forget all coordinates (e, g) where e is the contracted edge. Now the following conjecture seems natural.

Conjecture 8.4.9. *The variety $X(\mathcal{K}_{1,n}, G)$ is equal to the scheme-theoretic intersection of all the varieties $X(\mathcal{T}_i, G)$, where $\mathcal{T}_i$ are all prolongations of $\mathcal{K}_{1,n}$ which have both inner vertices of valency at least three. In other words, the sum of ideals of $X(\mathcal{T}, G)$ is the ideal of $X(\mathcal{K}_{1,n}, G)$.*

Remark 8.4.10. Since $X(\mathcal{K}_{1,n}, G)$ is a subvariety of $X(\mathcal{T}_i, G)$ for any prolongation $\mathcal{T}_i$ of $\mathcal{K}_{1,n}$, one inclusion is obvious. Note also that the condition of valency is necessary to make the conjecture non-obvious. Otherwise one of the varieties that we intersect would be equal to $X(\mathcal{K}_{1,n}, G)$, because a contraction of a vertex of degree 2 does not change the corresponding variety.

Let us explain how one will be able to compute phylogenetic invariants of a group-based model $X(\mathcal{T}, G)$ if Conjecture 8.4.9 holds. This algorithm requires using [SS05, Thm 23] (see also [Sul07, Thm 12]). It states that the ideal of phylogenetic invariants of a group-based model on $\mathcal{T}$ is generated by ideals of this model on $\mathcal{T}_1$ and $\mathcal{T}_2$ and some (easily computed) quadratic binomials, where $\mathcal{T}_1$ and $\mathcal{T}_2$ can be glued along petioles to give $\mathcal{T}$ as in Remark 8.1.7.
We first show how to compute phylogenetic invariants of $X(\mathcal{K}_{1,n}, G)$. Note that all prolongations $\mathcal{T}_i$ of $\mathcal{K}_{1,n}$ have maximal valency of vertices strictly smaller than $\mathcal{K}_{1,n}$. Hence the algorithm of computing phylogenetic invariants can run by induction on

this parameter. Each prolongation $\mathcal{T}_i$ of $\mathcal{K}_{1,n}$ can be constructed by gluing two claw trees $\mathcal{K}_{1,n_1}$ and $\mathcal{K}_{1,n_2}$ such that $n_1, n_2 < n$ along petioles. Thus, by [SS05, Thm 23], it is sufficient to compute phylogenetic invariants of $X(\mathcal{K}_{1,n_1}, G)$ and $X(\mathcal{K}_{1,n_2} G)$. Then, by Conjecture 8.4.9, we sum ideals of all prolongations. Working inductively, we obtain the result that the ideal of phylogenetic invariants of $X(\mathcal{K}_{1,n}, G)$ is generated by phylogenetic invariants of $X(\mathcal{K}_{1,3}, G)$ and some quadratic binomials.
Then one can compute phylogenetic invariants for any general group-based model $X(\mathcal{T}, G)$ for any tree $\mathcal{T}$ (without 2-valent vertices). Any tree $\mathcal{T}$ can be presented as a result of gluing some claw trees along petioles. Their phylogenetic invariants can be computed as above, and by [SS05, Thm 23] they generate phylogenetic invariants of $X(\mathcal{T}, G)$ together with some quadratic binomials.
In particular, if Conjecture 8.4.9 holds then the degree in which the ideals of claw trees are generated for a fixed group G cannot grow with the number of leaves. This means that $\phi(G) = \phi(G, 3)$, which can be computed in many cases. Therefore Conjecture 8.4.9 implies all these cases of Conjecture 8.4.2 in which we can compute $\phi(G, 3)$, including the most interesting 3-Kimura model.

Remark 8.4.11. One may observe that for a prolongation $\mathcal{T}_2$ of $\mathcal{T}_1$ are naturally contained in the same ambient space for any symmetric model of evolution, even if they do not correspond to toric varieties. Thus Conjecture 8.4.9 may prove helpful in computing phylogenetic invariants of claw trees for larger class of models than just general group-based models.

Example 8.4.12. Let us present the method of finding phylogenetic invariants in a simple case – we consider the binary Jukes-Cantor model on $\mathcal{K}_{1,4}$. This example is well-known and phylogenetic invariants of $X(\mathcal{K}_{1,4}, \mathbb{Z}_2)$ can be obtained with many different methods, but we have chosen this one because the number of phylogenetic invariants is small enough to be included in the paper.
Consider two prolongations of $K_{4,1}$ in Fig. 8.5.

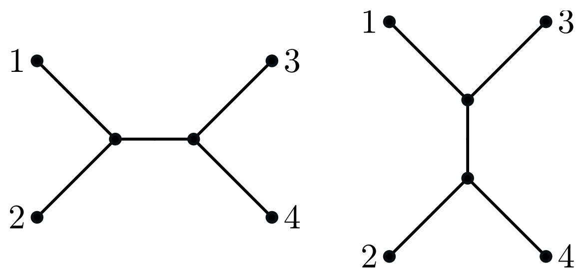


Figure 8.5: Prolongations of $\mathcal{K}_{1,4}$

There are 8 variables indexed by flows (or sockets) on $\mathcal{K}_{1,4}$:

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

Suppose that we already know the phylogenetic invariants for these prolongations. This particular case is very simple, but in general this is the step that follows from [SS05, Thm 23]. For the first prolongation the ideal is generated by two relations

$$q_{0000}q_{1111} - q_{1100}q_{0011}, \quad q_{1010}q_{0101} - q_{1001}q_{0110}.$$

For the other prolongation by suitably permuting variables we get the relations

$$q_{0000}q_{1111} - q_{1010}q_{0101}, \quad q_{1100}q_{0011} - q_{1001}q_{0110}.$$

These four relations (if fact one is redundant and it is enough to consider three of them) generate the ideal of $\mathcal{K}_{4,1}$.

One may probably think that Conjecture 8.4.9 is too strong to be true. However, we prove that it holds for the binary Jukes-Cantor model in Proposition 8.4.17. We also explain two modifications of this conjecture to weaker ones which can still have a lot of interesting applications.
The first states just that Conjecture 8.4.9 holds for large enough claw trees, which turns out to be equivalent to boundedness of phylogenetic complexity.

Proposition 8.4.13. *Fix an abelian group G. Conjecture 8.4.9 holds for $\mathcal{K}_{1,n}$ and G for n large enough if and only if function $\phi(n, G)$ is bounded.*

Proof. One implication is very easy. Suppose that Conjecture 8.4.9 holds for $n > n_0$. Let $m \in \mathbb{N}$ be such that ideals of $X(\mathcal{K}_{1,k}, G)$ are generated in degree m for $k \leq n_0$. Note that for $n > n_0$ the claw tree $\mathcal{K}_{1,n}$ can be constructed by gluing along petioles and contractions from a number of $\mathcal{K}_{1,k_i}$ for $k_i \leq n_0$. From the method of obtaining phylogenetic invariants described above we see that the ideal of $X(\mathcal{K}_{1,n}, G)$ is also generated in degree m, so $\phi(n, G) \leq m$.
For the other implication let us assume that $\phi(G) \leq m$. Consider a binomial B in the ideal of $X(\mathcal{K}_{1,n}, G)$, which is of degree less or equal to m. We need to prove that B belongs to the ideal of $X(\mathcal{T}, G)$, where $\mathcal{T}$ is a prolongation $\mathcal{T}$ of $\mathcal{K}_{1,n}$ (this is in fact even more than the statement of Conjecture 8.4.9). Such a binomial B can be expressed as a linear relation between (at most m) vertices of the polytope P_G associated to $(\mathcal{K}_{1,n}, G)$, see Theorem 8.1.5. Each vertex corresponds to a G-flow on $\mathcal{K}_{1,n}$. We write B as a pair of matrices A_1 and A_2 with elements of G as entries, where each column contains coordinates of a vertex of P_G, as in Observation 8.1.8. These matrices have at most m columns and exactly n rows.
Consider the matrix $A = A_1 - A_2$. Let us subdivide the first column of A into sets of at most $|G|$ elements summing up to the unit. This is possible, because when we look at partial sums a_1, $a_1 + a_2$, $a_1 + a_2 + a_3$, ..., $a_1 + \ldots + a_{|G|}$ of a sequence of $|G|$ elements of G, then either one of them is 0 or $a_1 + \ldots + a_j = a_1 + \ldots + a_k$ for some $j, k \leq |G|$, $j < k$, in which case $a_{j+1} + \ldots + a_k = 0$. This subdivision of the first column determines the subdivision of the set of rows of A into sets $R_1, \ldots, R_p$. Let us look now at the second column. In the same way we can subdivide it into sets of at most $|G|^2$ entries summing up to 0, and such that the entries in each set R_i from the subdivision in the previous step are all contained in one set of the new subdivision. Then, working inductively, we can subdivide the set of rows of A into

sets of at most $|G|^m$ elements such that in every column all entries from a set sum up to 0.

Hence for $n > |G|^m + 1$ we can find a set S of rows of A such that in each column entries of rows in S sum up to 0 (and entries of rows in the complement of S also) and both cardinality of S and of its complement are greater than 1. This implies that for every $i = 1, \ldots, m$ the sums of entries lying in the i-th column and in the rows in S are the same in A_1 and A_2. Therefore, when we add to both matrices an extra row whose entry in any column is equal to the sum of entries in this column and rows of S of A_1 or A_2, we obtain a representation of the binomial B on a prolongation of $\mathcal{K}_{1,n}$ – the added row corresponds to the added edge and S and its complement to petioles adjacent to its two vertices. □

Corollary 8.4.14. *In particular, this result implies that if Conjecture 8.4.3 (concerning the 3-Kimura model) holds then Conjecture 8.4.9 also holds for* $G \simeq \mathbb{Z}_2 \times \mathbb{Z}_2$ *for* $n > 257$. *In Section 8.4.3 we improve this estimate significantly.*

Remark 8.4.15. The argument in the proof of Proposition 8.4.13 can be easily generalized to the class of G-models.

Before we show the second weaker version of Conjecture 8.4.9, we explain another way of intersecting models of prolongations of $\mathcal{K}_{1,n}$, coming from toric geometry.

Let T_1 and T_2 be two subtori of a torus T with character lattice M. Then the character lattice M_i of T_i is isomorphic in a natural way with M/K_i, where K_i is a torsion free lattice corresponding to characters with trivial restriction to T_i. The ideal of T_i in $\mathbb{C}[T]$ is generated by binomials corresponding to relations between such characters. Points of T are given by semigroup homomorphisms $M \to \mathbb{C}^*$ and points of T_i are these homomorphisms which map K_i to 1. Then points of the intersection $T_1 \cap T_2$ are these homomorphisms $M \to \mathbb{C}^*$ which map the lattice $K_1 + K_2$ to 1.

The intersection Y of T_1 and T_2, possibly reducible, is given by the ideal corresponding to $K_1 + K_2$. This lattice may be non-saturated, but still Y contains a distinguished torus T', which is one of its connected components, whose character lattice is M/K', where K' is the saturation of $K_1 + K_2$. Let X_i be the toric variety that is the closure of T_i in the ambient projective space of T, and let X' be the closure of T'. We call the toric variety X' the **toric intersection** of X_1 and X_2.

The following conjecture is a variant of Conjecture 8.4.9 in which we consider the toric intersection instead of the scheme-theoretic intersection of models.

Conjecture 8.4.16. *Let* $\mathcal{T}_i$ *be all prolongations of* $\mathcal{K}_{1,n}$ *with two inner vertices of valency at least three. Then the toric variety* $X(\mathcal{K}_{1,n}, G)$ *is the toric intersection of all the toric varieties* $X(\mathcal{T}_i, G)$ *for any abelian group* G.

We state this conjecture, because it is much easier to check that the previous one – one has to look only at the tori of models. However, since all biologically meaningful points are contained in the big torus of the model (as explained in [CFS08]), such a result would be important from the point of view of applications. Moreover, it can be checked numerically for trees with small enough number of leaves. To explain it properly, let us consider the following general setting.

Assume that the tori T_i are associated with polytopes P_i and that T is just the big torus of the projective space $\mathbb{P}^s \supseteq T_i$. Let A_i be a matrix whose columns represent vertices of the polytope P_i. Characters which are trivial on T_i, or equivalently binomials in the ideal of corresponding to T_i, are represented by integer vectors in the kernel of A_i. The characters trivial on the intersection are given by integer vectors in $\ker A_1 + \ker A_2$. Note that the ideal of the toric intersection T' of the tori $T_i \subseteq T$ is generated by binomials corresponding to characters trivial on T', that is to elements of the saturated lattice of $\ker A_1 + \ker A_2$. These binomials define a toric variety in $\mathbb{P}^s$. This variety is contained in the intersection (in fact it is a toric component) of the toric varieties that are the closures of T_i. The equality may not hold however, as the intersection might be reducible.
In Conjecture 8.4.16 we have to compare two tori, one contained in the other: the big torus of $X(\mathcal{K}_{1,n}, G)$ and the torus of the toric intersection of $X(\mathcal{T}_i, G)$. To do this, it is sufficient to compare their dimension, that is the rank of the character lattice. Let us note that the dimension of the intersection of two tori $T_1 \cap T_2$ in $\mathbb{P}^s$ is given by $s - \operatorname{rank}(\mathbb{Z}^s \cap (\ker A_1 + \ker A_2))$. To compute this dimension it is enough to compute the ranks of matrices A_1, A_2 and B, where B is a matrix obtained by taking all rows of A_1 and A_2 (that is, $\ker B = \ker A_1 \cap \ker A_2$). This can be done very easily using standard functions of GAP (see [GAP12]).
We have applied this idea to check Conjecture 8.4.16 for a few trees with small number of leaves, which will be used in the next section.

8.4.3 Binary Jukes-Cantor and 3-Kimura models

To support Conjecture 8.4.9 we prove it in the case of the binary Jukes-Cantor model. This model is already well understood, it was investigated for example in [BW07, CP07, SS05]. In particular, the quadratic Gröbner basis is constructed explicitly for any tree in [CP07, Proposition 3]. Now we add the following result.

Proposition 8.4.17. *Conjecture 8.4.9 holds for the binary Jukes-Cantor model.*

Proof. We use the same notation as in the proof of Proposition 8.4.13, that is a binomial in the ideal of $X(\mathcal{K}_{1,n}, \mathbb{Z}_2)$ is represented by a pair of matrices A_1 and A_2, and we look at their difference $A = A_1 - A_2$. By [SS05, Thm 28] (see Proposition 8.4.4) we know that $\phi(\mathbb{Z}_2) = 2$. Hence it is sufficient to consider binomials of degree 2, i.e. A_1, A_2 and A have two columns, and prove that they come from prolongations of $\mathcal{K}_{1,n}$. For every such a binomial we construct a subset S of the set of rows of A which defines a suitable prolongation (i.e. entries in columns sum up to 0 and the cardinality of S and its complement is greater than 1).
Swapping columns of A_2 if necessary, we may assume the first row of A is $(0, 0)$. Let A' be the matrix obtained by deleting the first row of A. Note that, because each row of A_2 is a permutation of the corresponding row of A_1, rows of A are only $(0, 0)$ and $(1, 1)$. If A' contains a row $(0, 0)$ then we take S consisting of this row and the first row of A. And if there are only $(1, 1)$ rows in A' then we may take S consisting of two such rows. □

Remark 8.4.18. From the proof above it follows that in fact to obtain $X(\mathcal{K}_{1,n}, \mathbb{Z}_2)$ it is enough to intersect just three models of prolongations. For example, we may take prolongations corresponding to the subset S of the set of rows of A consisting of either the first two rows, or the first and the third row, or the second and the third one. If the first two options do not give a subset S satisfying the criteria, then the second and the third row must be equal.

We also prove a conditional result for the 3-Kimura model, improving the result noted in Corollary 8.4.14.

Proposition 8.4.19. *If Conjecture 8.4.3 (i.e. [SS05, Conj. 30]) holds then Conjecture 8.4.9 holds for $n > 8$.*

Proof. We again use the matrix notation to represent binomials in the ideal of phylogenetic invariants of $X(\mathcal{K}_{1,n}, \mathbb{Z}_2 \times \mathbb{Z}_2)$. Because we assume Conjecture 8.4.3, we consider matrices $A = A_1 - A_2$ with at most 4 columns. Since A is a difference of two matrices whose entries in each row are the same up to a permutation, all entries in each row sum up to $(0, 0) \in \mathbb{Z}_2 \times \mathbb{Z}_2$. Hence the number of 1's on the first coordinates of entries in each rows must be even, and the same applies to the second coordinates of entries.
Permuting the columns of A_2 if necessary, we may assume that all entries in the first row of A are $(0, 0)$. Let A' be the matrix obtained by deleting the first row of A. For each subset S of the set of rows of A' we consider the sum of rows in S, denoted by α_S. Note that each α_S also has an even number of 1's both on first coordinates and on second coordinates of entries. There are at most 64 such vectors (less if A has less than 4 columns).
By the pigeonhole principle, if $n > 8$ then we can find two subsets S_1 and S_2 of the set of rows of A' which are not complements of each other and such that $\alpha_{S_1} = \alpha_{S_2}$. If we take the symmetric difference of S_1 and S_2, we obtain a proper nonempty set S of rows of A' whose entries in each column sum up to $(0, 0)$. Finally, we add the first row of A either to S or its complement, so that both these sets have more than one element. Thus we obtain a subdivision of the set of rows of A which gives a prolongation $\mathcal{T}$ of $\mathcal{K}_{1,n}$ such that considered binomial is in the ideal of phylogenetic invariants of $(\mathcal{T}, \mathbb{Z}_2 \times \mathbb{Z}_2)$. □

Remark 8.4.20. For $n \leq 8$ we checked that the toric intersection of the 3-Kimura models on prolongations of $\mathcal{K}_{1,n}$ is $X(\mathcal{K}_{1,n}, \mathbb{Z}_2 \times \mathbb{Z}_2)$. We applied the linear algebra method described at the end of the previous section, and the computations were done using computer programs [GJ00, tt, GS, GAP12]. These results together with Proposition 8.4.19 prove that if Conjecture 8.4.3 holds, then also Conjecture 8.4.16 holds. Moreover, we have found it interesting that in all cases we checked it was sufficient to consider only two prolongations of $\mathcal{K}_{1,n}$.

We end with summarizing the results on relations, in the case of the 3-Kimura model, between the conjectures of [SS05] and these stated above.

Corollary 8.4.21. *For the 3-Kimura model Conjecture 8.4.9 implies both Conjectures 8.4.16 and 8.4.3 (i.e. [SS05, Conj. 30]). Moreover, Conjecture 8.4.3 implies 8.4.16, and also Conjecture 8.4.9 for $n > 8$.*

The topic of this section was further developed by Michałek in his doctoral thesis [Mic12b] and in [Mic11b, Mic12a]. Another recent interesting approach to bounding the degree of phylogenetic invariants, in a more general setting, is presented in [DE12].

Appendix

Here we present the precise results of our computations of Hilbert-Ehrhart polynomials for a few models (on the snowflake and 3-caterpillar trees), stated in Proposition 8.3.3. For $|G| \leq 7$ the numbers of lattice points in dilations nP are given for small values of n.
For $\mathbb{Z}_8$, $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ and $\mathbb{Z}_9$ given numbers are values of the Hilbert function and, since the first two of these models are not normal and for the last one we could not check the normality, we do not know if it is equal to the Ehrhart polynomial.

Models for $G = \mathbb{Z}_3$

n	*snowflake*	*3-caterpillar*
1	243	243
2	21627	21627
3	903187	904069
4	21451311	21496023
5	330935625	331976637
6	3647265274	3662146270
7	30770591364	30920349834
8	209116329075	210269891871
9	1189466778457	1196661601837
10	5831112858273	5868930577941
11	25205348411361	25377886917819

Models for $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ (3-Kimura)

n	*snowflake*	*3-caterpillar*
1	1024	1024
2	396928	396928
3	69248000	69324800
4	5977866515	5990170739
5	291069470720	291864710144
6	8967198289920	8995715702784

Models for $G = \mathbb{Z}_4$

n	*snowflake*	*3-caterpillar*
1	1024	1024
2	396928	396928
3	69248000	69324800
4	6122557220	6138552524
5	310273545216	311525688320
6	10009786400352	10062179606880

Models for $G = \mathbb{Z}_5$

n	*snowflake*	*3-caterpillar*
1	3125	3125
2	3834375	3834375
3	2229584375	2230596875
4	640338121875	642089603125

Models for $G = \mathbb{Z}_7$

In this case the first three dilations of polytopes corresponding to considered models have the same number of lattice points. The numbers of lattice points in the fourth dilations were too big to obtain precise results without a lot of changes in the program. Hence we computed only their values modulo 64, which is sufficient to prove that the Hilbert-Ehrhart polynomials are different.

n	*snowflake*	*3-caterpillar*
1	16807	16807
2	117195211	117195211
3	423913952448	423913952448
4	$\equiv 54 \mod 64$	$\equiv 14 \mod 64$

Models for $G = \mathbb{Z}_8$

n	*snowflake*	*3-caterpillar*
1	32768	32768
2	454397952	454397952
3	3375180251136	3375013036032

Models for $G = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$

n	*snowflake*	*3-caterpillar*
1	32768	32768
2	454397952	454397952
3	3375180251136	3375013036032

Models for $G = \mathbb{Z}_9$

n	*snowflake*	*3-caterpillar*
1	59049	59049
2	1499667453	1499667453
3	20938605820263	20937202945056

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