Phylogenetic invariants for $\mathbb{Z}_3$ scheme-theoretically

Maria Donten-Bury

Abstract. We study phylogenetic invariants of models of evolution with group of symmetries $\mathbb{Z}_3$. We prove that projective schemes corresponding to the ideal $I$ of phylogenetic invariants of such a model and to its subideal $I'$ generated by elements of degree at most 3 are the same. This is motivated by a conjecture of Sturmfels and Sullivant [SS05, Conj. 29], which would imply that $I = I'$.

1. Introduction

One of the most important questions in phylogenetic algebraic geometry, motivated by applications, is to determine the ideal of phylogenetic invariants, i.e. the ideal of polynomials vanishing on an algebraic variety corresponding to a model of evolution. It turns out that even determining the minimal degree in which this ideal is generated is a difficult problem. It is often considered in the case of the class of general group-based models of evolutions (see e.g. [SS03, Sect. 8.10]): a part of the structure of such a model is an abelian group $G$ of symmetries. The simplest (but having very interesting properties, studied in [BW07]) example of this class is the binary model, $G \cong \mathbb{Z}_2$. The Kimura 3-parameter model with $G \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ is its generalization, important from the point of view of motivation coming from computational biology. Another small example is the model with $G \cong \mathbb{Z}_3$, considered in this note. It is known that algebraic varieties associated with group-based models (i.e. their geometric models) are toric, [SSE93, SS05]. This class appears also in connection with theoretical physics, see [Man09].

In [SS05, Conj. 29] Sturmfels and Sullivant conjecture that the ideal of phylogenetic invariants for a group-based model with group of symmetries $G$ is at most $|G|$. A very important case of the Kimura 3-parameter model is referred to in a separate conjecture, [SS05, Conj. 30]. The authors give a proof for the binary model and provide some experimental data supporting the conjecture for small trees and groups. In [DBM12] we analyze a few more examples with computational methods, and also suggest a geometric approach to the problem of determining phylogenetic invariants.

Let $I$ be the ideal of phylogenetic invariants for a tree $T$ and an abelian group $G$ and $I'$ be the ideal generated by the invariants in degree at most $|G|$. If [SS05]
Conj. 29] is true, it implies that $I = I'$. Since comparing these two ideals is a hard task, there has been a few attempts to compare geometric objects defined by them: projective schemes, sets of zeroes, or even sets of zeroes in the open orbit in cases where the model is a toric variety. This last approach is presented in [CFSM14]. The set-theoretical version of this conjecture for the class of equivariant models introduced in [DK09] is considered in [DE12]. In [Mic13] Michalek proves the scheme-theoretical version for the 3-Kimura model, and also that for a fixed abelian group $G$ there is a bound on the degree in which $I$ is generated, independent on the size of the tree.

The aim of this note is to give a combinatorial proof of the scheme-theoretic version for $G \simeq \mathbb{Z}_3$, using ideas similar to these presented in [Mic13].

**Theorem 1.1.** For $G \simeq \mathbb{Z}_3$ and any tree the projective schemes defined by the ideal $I$ of phylogenetic invariants of the corresponding model and its subideal $I'$ generated by elements of degree 2 and 3 are the same. That is, the saturation of $I'$ with respect to the irrelevant ideal is generated in degree 3.

Note that this result implies also the set-theoretic one: to check whether a point lies in the set of zeroes of the ideal of phylogenetic invariants for $\mathbb{Z}_3$ it is sufficient to see if the invariants of degree 3 vanish.

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**2. Idea of the proof**

The construction of phylogenetic invariants for group-based models (or, more generally, equivariant models) can be reduced to the case of claw trees $K_{1,r}$ (trees with one inner vertex and $r$ leaves), see e.g. [SS05, Sect. 5] and [Sul07]. From now on, let $I$ be the ideal of phylogenetic invariants on a chosen claw tree $K_{1,r}$ and $I'$ be the ideal generated by the invariants in degree at most $|G|$.

We use the notation of [Mic13, Sect. 3] for the elements of $I$ and $I'$, i.e. we present them as relations between group-based flows (see [Mic13, Def. 3.5]) on the tree.

**Definition 2.1.** A group-based flow is a function $n: E_T \rightarrow G$, i.e. an assignment of group elements to the edges of the tree $T$, such that for any inner vertex $v$ of $T$ and all edges $e_1, \ldots, e_k$ adjacent to $v$ we have $n(e_1) + \cdots + n(e_k) = 0$.

For $K_{1,r}$ we may identify the set of edges with $\{1, \ldots, r\}$, so a group-based flow is just a function $n: \{1, \ldots, r\} \rightarrow G$ such that all its values sum up to 0.

By [Mic11], group-based flows correspond to vertices of the lattice polytope describing the toric structure of the associated geometric model (as in [CLST11, Chapter 2]). Then, using [Stu96, Lem. 4.1], we can express generators of the saturation of $I'$ as relations $\sum L = \sum R$, where $L$ and $R$ are sets of group-based flows (we assume $L \cap R = \emptyset$). We add flows coordinatewise, counting different group elements at each index. By adding sufficiently many copies of trivial flow (which corresponds to saturation), denoted by 0, we may assume that $L$ and $R$ consist only of flows of two types:

1. pairs – the flow with only two nontrivial entries,
2. triples – the flow with only three nontrivial entries.
This is a consequence of a more general statement, see [Mic11, Lem. 7.2], but in the case of $\mathbb{Z}_3$ (and other groups of small order) the set of possible basic configurations is relatively simple and allows us to proceed with the combinatorial argument. Let $g_1, g_2$ be the nontrivial elements of $\mathbb{Z}_3$. There is one type of pairs and two types of triples:

1. $g_1$ and $g_2$ assigned to two chosen indices $a$ and $b$ respectively – will be denoted $(a, b)$;
2. $g_1$ assigned to three chosen indices $a$, $b$ and $c$ – will be denoted $(a, b, c)_{g_1}$;
3. $g_2$ assigned to three chosen indices $a$, $b$ and $c$ – will be denoted $(a, b, c)_{g_2}$.

Note that for the pair the order of $a$ and $b$ is meaningful, while for the triples a permutation of $(a, b, c)$ does not change anything. Obviously, indices in a pair or a triple must be different.

Moreover, we may assume that on one side there appears only one type of triples.

**Lemma 2.2.** If $R$ or $L$ contains both a $g_1$-triple $(a, b, c)_{g_1}$ and a $g_2$-triple $(x, y, z)_{g_2}$, we may replace them with pairs.

**Proof.** We use the relation

$$(a, b, c)_{g_1} + (x, y, z)_{g_2} + 0 = (a, x) + (b, y) + (c, z).$$

This may require adding a trivial flow to both sides of the relation if there is no at the side we modify. Also, it may be necessary to permute entries of a triple so that we obtain sensible pairs (i.e. with different indices), but such a permutation always exists. This way we decompose the chosen element $\sum L = \sum R$ (with some trivial flows added) into a sum of an element of $I'$ (a relation of degree 3 multiplied by something) and a relation with smaller number of triples. Hence we reduce our relation in a finite number of steps to the form where on each side of the relation there are only $g_1$-triples or only $g_2$-triples.

The general idea of the argument is the induction, but not on the standard degree, because we need to multiply the relation by the variable corresponding to the trivial flow in Lemma 2.2. We can use for example the grading by the size of the flow: a variable is in the $d$-th gradation if the corresponding flow has $d$ nontrivial entries. We will take a relation and decompose it into a sum of relations in $I'$, i.e. relations of (standard) degree 2 or 3 multiplied by something, and relations of smaller degree with respect to the grading introduced above. Before starting the induction we change the relation such that there are no $g_1$-triples and $g_2$-triples together on one side, by Lemma 2.2. We will always assume that this is satisfied and ensure that our modifications do not violate this condition. In the remaining sections we consider a few separate cases depending on possible configurations of elements in $L$ and $R$.

### 3. No pairs

First assume that $L$ and $R$ consist only of triples and without loss of generality we may assume that there are only $g_1$-triples (we will use the symmetry between $g_1$ and $g_2$, and also between $L$ and $R$, all the time).

It is worth noting that the fact that in this case the relations can be generated in degree 2 is a consequence of a result on uniform (or, much more generally, strongly base orderable) matroids. This is a special case of the White’s conjecture, for the details see [LM14] and references therein.
3.1. There are \(g_1\)-triples with two indices in common. Say \((1, 2, 3)_{g_1} \in L\) and \((1, 2, a)_{g_1} \in R\) (we permute the indices if necessary). Then there is \((3, b, c)_{g_1} \in R\), because \(g_1\) appears in \(L\) at the index 3. If \(a \neq b\) and \(a \neq c\), then we can use the relation

\[(1, 2, a)_{g_1} + (3, b, c)_{g_1} = (1, 2, 3)_{g_1} + (a, b, c)_{g_1},\]

and reduce the flow \((1, 2, 3)_{g_1}\). By this reduction we obtain a relation of smaller degree with respect to the considered grading. Hence we may assume that \((3, a, c)_{g_1} \in R\) for some \(b\). More generally, every appearance of \(g_1\) at the index 3 in \(L\) gives a triple of type \((3, a, c)_{g_1}\) in \(R\) and 3 can appear in \(g_1\)-triples only of this type.

Symmetrically, every appearance of \(g_1\) on the index \(a\) in \(R\) gives a triple of type \((a, 3, c)_{g_1}\) in \(L\) and \(a\) can appear in \(L\) only in \(g_1\)-triples of this type.

We finish with an argument which will be repeated frequently throughout the proof. Assume that there are \(n\) \(g_1\)-triples containing \(3\) in \(R\). All of them contain \(a\). Then \(a\) appears at least \(n + 1\) times with \(g_1\) in \(R\), in all triples with 3 and in \((1, 2, a)_{g_1}\), hence also in \(L\). But this means that 3 appears at least \(n + 2\) times with \(g_1\) in \(L\): in \((1, 2, 3)_{g_1}\) and \(n + 1\) times together with \(a\). This is a contradiction, since the numbers of appearances of \(g_1\) on a chosen index on both sides must be equal.

Let us reformulate this in a form of a general observation, so we can refer to it later on.

**Lemma 3.1.** Assume that each occurrence of some \(\alpha\) in \(S_1 \in \{L, R\}\) with \(g_m\) induces an occurrence of \(\beta\) in \(S_1\) with \(g_k\), and also each occurrence of \(\beta\) in \(S_2 \in \{L, R\}\), \(S_2 \neq S_1\), with \(g_k\) induces an occurrence of \(\alpha\) in \(S_2\) with \(g_m\). Then \(\beta\) cannot appear in \(S_1\) with \(g_k\) in a different configuration than the one induced by the occurrence of \(\alpha\) with \(g_m\).

**Proof.** Counting appearances of \(\alpha\) with \(g_m\) and \(\beta\) with \(g_k\), exactly as in the example above. \(\square\)

3.2. There are no triples \(\alpha \in L, \beta \in R\) with two indices in common.

Take \((1, 2, 3)_{g_1} \in L\), then there is some \((1, a, b)_{g_1} \in R\). If there is \((2, c, d)_{g_1} \in R\) such that \(\{a, b\} \neq \{c, d\}\), then we can find a relation which gives a reduction to the previous case. For example, if \(a \notin \{c, d\}\), then the relation used is \((1, a, b)_{g_1} + (2, c, d)_{g_1} = (1, 2, b)_{g_1} + (a, c, d)_{g_1}\). Hence we may assume that 2 with \(g_1\) goes always in a triple \((2, a, b)_{g_1}\) in \(R\). Using the same argument we prove that 3 with \(g_1\) goes always in the triple \((3, a, b)_{g_1}\) in \(R\).

Then \(a\) and \(b\) appear in \(g_1\)-triples in \(L\). By the same argument as above, \(a\) appears with \(g_1\) in \(L\) always in \((a, 2, 3)_{g_1}\) and \(b\) in \((b, 2, 3)_{g_1}\). We finish in a very similar way as in Lemma 3.1, we just have to consider appearances of \(g_1\) at both indices 2 or 3 in \(R\) and at \(a\) and \(b\) in \(L\).

4. At least two pairs on one side, four different indices

Now assume that \((1, 2) \in L\) and \((a, b) \in L\) such that \(1, 2, a, b\) are all different (we swap \(L\) with \(R\) if necessary).

**Remark 4.1.** If two pairs \((1, 2)\) and \((a, b)\) with all indices different occur on one side of the relation, then we may swap their elements, that is exchange them with \((1, b)\) and \((a, 2)\) by applying quadric relation \((1, 2) + (a, b) = (1, b) + (a, 2)\).

There are three cases to consider (up to swapping \(g_1\) and \(g_2\)):
(2.1) \( R \) contains triples \((x, y)_{g_1}\) and \((a, s, t)_{g_1}\) and 2 and \(b\) are not contained in any \(g_2\)-triple in \(R\):

(2.2) \( 1 \) is contained in a \(g_1\)-triple in \(R\), \(a\) does not appear in any \(g_1\)-triple in \(R\) and 2 and \(b\) do not appear in any \(g_2\) triple in \(R\):

(2.3) there are no \(g_1\)-triples containing one of \(a\) and no \(g_2\)-triples containing \(2, b\) in \(R\).

4.1. There are \((1, x, y)_{g_1}, (a, s, t)_{g_1}, (u, 2)\) and \((v, b)\) in \(R\). If \(u \notin \{x, y\}\) or \(v \notin \{s, t\}\) then we could use a relation to get \((1, 2)\) or \((a, b)\) in \(R\). Hence we may assume that \(u = x\) and \(v = s\). Now, \(x\) appears with \(g_1\) in \(L\).

4.1.1. First assume that it occurs only in triples, that is \((x, c, d)_{g_1} \in L\). Then either we can use the relation \((1, 2) + (x, c, d)_{g_1} = (x, 2) + (1, c, d)_{g_1}\) and reduce \((x, 2)\) or we may assume that \(c = 1\). In the latter case \(1\) appears with \(g_1\) in \(R\) more times.

Assume it is in a pair \((1, e) \in R\). Then we may use quadric relations between pairs in \(L\) and \(R\) to obtain a reduction of a pair, unless \(x = s = e\), which means that \((a, x, t)_{g_1} \in R\). But, using the relation \((1, x) + (a, x, t)_{g_1} = (t, x) + (a, x, 1)_{g_1}\) we may assume that \((a, x, 1)_{g_1} \in R\). And in \(L\) either we use the relation \((a, b) + (x, 1, a)_{g_1} = (x, b) + (a, 1, d)_{g_1}\), which allows us to reduce \((x, b)\), or \(a = d\) and \((x, 1, a)_{g_1}\) can be reduced.

If \(1\) appears with \(g_1\) in \(R\) only in triples, we have \((1, e, f)_{g_1} \in R\). Then either we can use the relation \((x, 2) + (1, e, f)_{g_1} = (1, 2) + (x, e, f)_{g_1}\) and reduce \((1, 2)\) or we may assume that \(e = x\). But then we get a contradiction by Lemma 5.1 applied to the occurrences of \(1\) and \(x\) with \(g_1\).

4.1.2. The second possibility is that \(x\) appears with \(g_1\) in \(L\) in a pair \((x, c)\). If \(c \neq 1\) then we use the relation \((x, e) + (1, 2) = (x, 2) + (1, c)\) and reduce \((x, 2)\), so we may assume that \((x, 1) \in L\). Then \(1\) appears in \(R\) with \(g_2\), and it can be only in pairs by Lemma 2.2. Then \((e, 1) \in R\), and in fact this pair must be equal to \((2, 1)\), because otherwise we would use the relation \((e, 1) + (x, 2) = (x, 1) + (e, 2)\) and reduce \((x, 1)\).

Now we try to apply the cubic relation

\[(x, 2) + (s, b) + (2, 1) = (x, 1) + (2, b) + (s, 2)\]

in \(R\) and reduce \((x, 1)\). This fails only if \(s = 2\). In this case, if a pair \((2, b) \in L\) then we swap elements with either \((a, b)\) or \((x, 1)\) (see Remark 4.1) and reduce \((2, 1)\) or \((2, b)\). This fails only if \(x = h = a\), but then \((a, 2) \in L\) and the same pair can be obtained in \(R\) by swapping elements of \((1, 2)\) and \((a, b)\). And if there is a triple \((2, i, j)_{g_1} \in L\), then we try to use the relations

\[(2, i, j)_{g_1} + (a, b) = (a, i, j)_{g_1} + (2, b)\]

and reduce \((2, b)\) or \((2, 1)\).

This is impossible only if \(\{i, j\} \supseteq \{x, a\}\). Since we already excluded the case \(x = a\), we have \((2, x, a)_{g_1} \in L\). In \(R\) we use the relation \((a, 2, t)_{g_1} + (x, 2) = (x, a)_{g_1} + (t, 2)\) (note that \(t \neq 2\) since they appear in the same triple), which allows us to reduce \((2, x, a)_{g_1}\).

4.2. Now \(1\) is contained in some \(g_1\)-triple in \(R\), say \((1, x, y)_{g_1}\), and \(a\) does not appear in any \(g_1\)-triple and \(2, b\) in any \(g_2\)-triple in \(R\). Then \(a\) appears with \(g_1\) and 2 and \(b\) with \(g_2\) in \(R\) only in pairs. Take such a pair \((z, 2)\).

Then \(z \in \{x, y\}\), because otherwise we could use the relation \((1, x, y)_{g_1} + (z, 2) =\)
and reduce either $(x, y)_g, (1, 2)$; assume $z = x$. Take now $(a, u)$ and $(v, b)$. Then $u = v$, because otherwise the relation $(a, u) + (v, b) = (a, b) + (v, u)$ would allow us to reduce $(a, b)$. Moreover, $u = x$ because of the relations $(a, u) + (x, 2) = (a, 2) + (x, u)$ in $R$ and $(1, 2) + (a, b) = (1, b) + (a, 2)$ in $L$. Summing up, $R$ contains $(1, x, y)_g, (x, 2), (a, x)$ and $(x, b)$. Let us determine in what configurations $x$ appears with $g_1$ in $L$. If in a pair $(x, c)$ then we can use one of the relations

$$(x, c) + (1, 2) = (x, 2) + (1, c)$$

and reduce $(x, 2)$ or $(x, b)$. Hence we may assume it appears only in triples. If $(x, c, d)_{g_1}$ is such a triple then we try to use the relations

$$(x, c, d)_{g_1} + (1, 2) = (x, 2) + (1, c, d)_{g_1}$$

and reduce the same pairs as before. It fails only if $\{c, d\} = \{1, a\}$, so we may assume that $x$ appears with $g_1$ in $L$ only in triples $(x, 1, d)_{g_1}$. But then we can use the relation $(1, x, y)_{g_1} + (a, x) = (1, x, a)_{g_1} + (y, x)$ in $R$, which works because $x \neq y$ as they appear in the same triple, and reduce $(x, y, z)_{g_1}$.

4.3. We assume that 1, a do not appear in any $g_1$-triples and 2, b in any $g_2$-triples in $R$. There are pairs $(1, x), (x', 2), (a, y)$ and $(y', b)$ in $R$. Then we may assume that $x = x'$ and $y = y'$, because otherwise we could use a relation of degree 2 to produce a pair $(1, 2)$ or $(a, b)$ and reduce it with equal pair in $L$. Then, if $x \neq y$, we could use the relation $(1, x) + (y, b) = (1, b) + (x, y)$ in $R$ and the relation $(1, 2) + (a, b) = (1, b) + (2, a)$ in $L$ and reduce $(1, b)$. Hence we assume that $R$ contains pairs $(1, x), (x, 2), (a, x)$ and $(x, b)$. Let us check in what configurations $x$ appears in $L$. If it appears in a pair $(x, c)$ then we could use one of the relations

$$(x, c) + (1, 2) = (x, 2) + (1, c)$$

and reduce either $(x, 2)$ or $(x, b)$, as before. Hence we may assume that $x$ does not appear with $g_1$ in any pair in $L$ and also, arguing in the same way, we may assume $x$ does not appear with $g_2$ in any pair in $L$. This means that $L$ must contain a $g_1$-triple and a $g_2$-triple with $x$, but by Lemma 2.2, such a situation cannot happen.

5. At least two pairs on one side, three different indices

Now we assume there are no two pairs consisting of four different indices, but there are two such that the set of indices has three elements. Let 1, 2 and $a$ be different indices. There are two cases (up to swapping $g_1$ and $g_2$):

3.1) $L$ contains pairs $(1, 2), (1, a)$.

3.2) $L$ contains pairs $(1, 2), (a, 1)$.

5.1. Case $(1, 2), (1, a)$. There are three different possibilities to consider:

3.1.1) 2 or $a$ appear in $g_2$-triples in $R$;

3.1.2) 1 appears in a $g_1$-triple in $R$;

3.1.3) 1 does not appear in any $g_1$-triple in $R$ and 2, $a$ do not appear in any $g_2$-triples in $R$. 
5.1.1. Assume that $R$ contains a triple $(2, x, y)_{g_2}$ and a pair $(1, t)$. Then we try to use the relation $(2, x, y)_{g_2} + (1, t) = (t, x, y)_{g_2} + (1, 2)$ and reduce $(1, 2)$. Consider the situation when it is impossible: let $x = t$ and $(1, x) \in R$. We may assume $x \neq a$, otherwise we get an immediate reduction. Now consider flows with $x$ in $L$. If $x$ appears with $g_2$ in $L$ in a pair $(c, x)$ then we may swap elements in pairs as in Remark 4.1, hence $(1, x), c, d$ and reduce $(1, x)$, because either $c \neq 2$ or $c \neq a$. Hence we may assume that $x$ appears with $g_2$ in $L$ just in triples.

Let $(x, c, d)_{g_2} \in L$. Then either we use one of the relations

$$(x, c, d)_{g_2} + (1, 2) = (2, c, d)_{g_2} + (1, x)$$

and reduce $(1, x)$ or every $g_2$-triple in $L$ containing $x$ is of the form $(x, a, 2)_{g_2}$. Now we check in what configurations 2 can occur in $R$ with $g_2$. If it occurs only in triples, then for $(2, e, f)_{g_2} \in R$ we try to use the relation $(2, e, f)_{g_2} + (1, x) = (x, e, f)_{g_2} + (1, 2)$ and reduce $(1, 2)$. It is impossible only in the case where all $g_2$-triples in $R$ containing 2 contain also $x$, but then we finish the argument by applying Lemma 4.1 to occurrences of 2 and $x$ with $g_2$.

This leaves us in a situation where there is $(e, 2) \in R$. Then we may assume that $e = x$, because otherwise we swap elements in pairs in $R$ and reduce $(1, 2)$. But then $x$ occurs with $g_1$ in $L$ and it has to be in a pair since we already have $g_2$-triples there. If $(x, f) \in L$ and $f \neq 1$ then we swap indices with $(1, 2)$ and reduce $(x, 2)$. And if $(x, 1) \in L$ then we use the relation $(x, a, 2)_{g_2} + (x, 1) = (x, a, 1)_{g_2} + (x, 2)$, hence $(x, 2)$ can also be reduced.

5.1.2. In $R$ there are $(1, x, y)_{g_1}, (z, 2)$ and $(t, a)$. We may assume that $z = x$, because if not then we could use the relation $(1, x, y)_{g_1} + (z, 2) = (z, x, y)_{g_1} + (1, 2)$ and reduce $(1, 2)$. (In the same way $t \in \{x, y\}$, we will use it later.)

First assume that both $x$ and $t$ occur in $L$ with $g_1$ in a pair, i.e. $(x, c), (t, d) \in L$. Then we can swap elements in pairs as in Remark 4.1 and reduce a pair, unless $c = d = 1$. But in this case we have $(c, 1) \in R$, because 1 cannot appear in a $g_2$-triple in $R$, since there is already a $g_1$-triple. This allows us to swap elements in pairs and reduce $(x, 1)$ or $(t, 1)$.

Hence the only possibility is that $x$ or $t$ occurs in $L$ with $g_1$ only in triples – let $x$ have this property. If $(x, f, h)_{g_1} \in L$ then we try to use the relation $(x, f, h)_{g_1} + (1, 2) = (1, f, h)_{g_1} + (x, 2)$ and reduce $(x, 2)$. This fails only if every $g_1$-triple in $L$ containing $x$ contains 1. Consider possible flows with $g_1$ at index 1 in $R$.

If all of them are triples then we may assume that they contain $x$, because otherwise the relation $(1, i, j)_{g_1} + (x, 2) = (x, i, j)_{g_1} + (1, 2)$ can be applied and we have a reduction of $(1, 2)$. In this case the argument is finished by Lemma 3.1 applied to occurrences of 1 and $x$ with $g_1$.

We are left with the case when 1 appears with $g_1$ in $R$ in a pair $(1, k)$. We try to swap elements in pairs in $R$ and reduce $(1, 2)$ or $(1, a)$, which fails only if $k = x = t$.

But then we have $(1, x) \in R$ and $x$ occurs in $L$ with $g_2$, and it can be only in a pair because there already is a $g_1$-triple. Hence take $(m, x) \in L$. Now we can swap elements in pairs in $L$ in a way which allows to reduce $(1, x)$.

5.1.3. Here 1 does not appear in any $g_1$-triple in $R$ and 2, a do not appear in $g_2$-triples in $R$. Hence $R$ contains pairs $(1, x), (y, 2)$ and $(z, a)$. If $x \neq y$ or $x \neq z$ we can use one of the relations

$$(1, x) + (y, 2) = (1, 2) + (y, x)$$

$$(1, x) + (z, a) = (1, a) + (z, x)$$
and reduce (1, 2) or (1, a). So we may assume that \( R \) contains (1, x), (x, 2) and (x, a). We see that \( x \) appears with \( g_1 \) in \( L \). If it appears in a pair \((x, c)\) such that \( c \neq 1 \) then we can use the relation \((x, c) + (1, 2) = (x, 2) + (1, c) \) and reduce \((x, 2)\).

Hence if \( x \) appears with \( g_1 \) in \( L \) in a pair then it is \((x, 1)\).

If such a pair belongs to \( L \) then 1 must appear with \( g_2 \) in \( R \). If there is \((1, s, t)_{g_2} \in R\) then we try to use the relation \((1, s, t)_{g_2} + (x, 2) = (2, s, t)_{g_2} + (x, 1)\) and reduce \((x, 1)\). It fails only if \( 2 \in \{s, t\} \), but this situation contradicts the assumption that 2 does not appear in \( g_2\)-triples in \( R \). So there must be some \((s, 1) \in R\). But in this case we can use one of the relations

\[(s, 1) + (x, 2) = (x, 1) + (s, 2) \quad \text{and reduce } (x, 1).\]

Therefore we are left with the case where \( x \) appears with \( g_1 \) in \( L \) only in triples; there must be at least one such triple.

Then, because \((1, x) \in R\), we know that \( x \) appears also with \( g_2 \) in \( L \). It cannot be in a \( g_2\)-triple since we already have \( g_1\)-triples in \( L \), so it appears in a pair \((c, x)\).

We can use one of the relations

\[(c, x) + (1, 2) = (c, 2) + (1, x) \quad \text{and reduce } (1, x).\]

5.2. Case \((1, 2), (a, 1)\). First two cases are situations when at least one of \(\{1,2,a\}\) occurs in a triple in \( R \). Because of Lemma 2.2 up to swapping \( g_1 \) with \( g_2 \) there are just two different possibilities. In the last case we see what happens when there are no such triples.

Remark 5.1. If on one side there are pairs \((\alpha, \beta), (\gamma, \alpha)\), then either all the remaining pairs are equal to those or \((\beta, \gamma)\), or we are in the situation which was already considered in section 2 (four different indices in pairs) or 3.1 (an index repeats with the same value in two different pairs).

5.2.1. First consider the case when for the pair \((1, 2)\) the first element appears in a \( g_1 \)-triple in \( R \) and the second does not appear in a \( g_2 \)-triple in \( R \). So \( R \) contains a triple \((1, x, y)_{g_1}\) and a pair \((z, 2)\). The relation \((1, x, y)_{g_1} + (z, 2) = (z, x, y)_{g_1} + (1, 2)\), which leads to the reduction of \((1, 2)\), cannot be used only if \( z \in \{x, y\} \), so we may assume that 2 appears with \( g_2 \) in \( R \) only in pairs \((x, 2)\) (by Remark 5.1 \( y, 2 \notin R \)).

Also, 1 appears in \( R \) with \( g_2 \) and it has to be only in pairs, since there already are \( g_1 \)-triples. If \((s, 1) \in R\) then either, by Remark 5.1 we are in one of the previous cases or it must be equal to \((2, 1)\) (because \( x \neq 1 \)). Hence we assume that \((2, 1) \in R\).

Then 2 appears in \( L \) with \( g_1 \). If in a pair, then by Remark 5.1 it is \((2, a)\) and we use the cubic relation

\[(1, 2) + (a, 1) + (2, a) = (1, a) + (2, 1) + (a, 2)\]

in \( L \) and reduce \((2, 1)\).

Thus we only have to consider the case when 2 appears with \( g_1 \) in \( L \) just in triples.

Take such a triple \((2, c, d)_{g_1}\). If \( a \notin \{c, d\} \) then we use the relation \((2, c, d)_{g_1} + (a, 1) = (a, c, d)_{g_1} + (2, 1)\) and reduce \((2, 1)\), so we may assume that if 2 appears in \( L \) with \( g_1 \) then this is always in a triple containing \( a \).

If \( a \) appears in \( R \) with \( g_1 \) in a pair \((a, t)\), then by Remark 5.1 this must be equal to \((x, 2)\) (because \( a \notin \{1, 2\} \)). In particular, \( x = a \) and \( R \) contains \((1, a, y)_{g_1}\); recall that \((2, a, d)_{g_1} \in L \). We use the following relations in \( L \) and \( R \) respectively:

\[(2, a, d)_{g_1} + (1, 2) = (2, a, 1)_{g_1} + (d, 2) \quad (1, a, y)_{g_1} + (2, 1) = (1, a, 2)_{g_1} + (y, 1)\]
and reduce the triple. The last possibility is that $a$ appears in $R$ with $g_1$ just in triples and let $(a, s, t)_{g_1}$ be such a triple. Then either we can use the relation $(a, s, t)_{g_1} + (2, 1) = (a, 1) + (2, s, t)_{g_1}$ and reduce $(a, 1)$, or all such triples contain also $2$, in which case we get a contradiction by Lemma 3.1 used to occurrences of $2$ and $a$ with $g_1$.

5.2.2. Now consider the case when $1$ does not appear in a $g_1$-triple and $2$ appears in a $g_2$-triple in $R$. So $R$ contains a pair $(1, x)$ and a triple $(2, y, z)_{g_2}$. If $x \notin \{y, z\}$ then we can use the relation $(1, x) + (2, y, z)_{g_2} = (1, 2) + (x, y, z)_{g_2}$ and reduce $(1, 2)$, so we may assume that $x = z$ and $(2, x, y)_{g_2} \in R$. Now $a$ must appear with $g_1$ in $R$. It cannot be in a triple since there are $g_2$-triples already, so we have some $(a, s) \in R$. If $s = 1$ then $(a, 1)$ can be reduced, and if not, by Remark 5.1 we obtain $x = a$, i.e. $R$ contains $(1, a), (a, s)$ and $(2, a, y)_{g_2}$. If $1$ appears with $g_2$ in $R$ in a pair $(c, 1)$ then by Remark 5.1 we have $c = s$ and we use the relation

$$(1, a) + (a, s) + (s, 1) = (1, s) + (a, 1) + (s, a)$$

in $R$ and reduce $(a, 1)$. If it appears in a triple $(1, d, e)_{g_2}$ and $s \notin \{d, e\}$ then we use the relation $(1, d, e)_{g_2} + (a, s) = (a, 1) + (s, d, e)_{g_2}$ and reduce $(a, 1)$ again. Hence we may assume that $1$ occurs with $g_2$ in $R$ only in triples containing $s$. Then we look at $a$ with $g_2$ in $L$. If it occurs in a pair $(f, a)$, then by Remark 5.1 $f = 2$, so we again use the cubic relation between pairs and reduce $(1, a)$. Thus we may assume that $a$ occurs with $g_2$ in $L$ only in triples. Moreover, if $(a, h, i)_{g_2}$ is such a triple, then either we use the relation $(a, h, i)_{g_2} + (1, 2) = (2, a, y)_{g_2}$ and reduce $(1, 2)$, or we may assume that such a triple always contains $2$. Thus $2$ occurs more times with $g_2$ in $R$. If it is only in triples then, because $x = a$, by the argument at the beginning of 5.2.2 we may assume that such a triple always contains also $a$. In this last case we finish by Lemma 3.1 applied to occurrences of $2$ and $a$ with $g_2$. And if there is a pair $(m, 2) \in R$, then by Remark 2.2 we have $s = 2$ and in particular $(a, 2), (1, 2, e)_{g_2} \in R$. Then we use the following relations in $L$ and $R$ respectively

$$(a, 2, i)_{g_2} + (a, 1) = (a, 2, 1)_{g_2} + (a, i)$$

and reduce $(a, 2, 1)_{g_2}$.

5.2.3. Here we assume that $1$ appears only in pairs in $R$, and $2$ with $g_2$ and $a$ with $g_1$ also appear only in pairs in $R$. So in $R$ there are pairs $(1, x), (x', 2), (y, 1)$, and $(a, y')$. If $x \neq x'$ or $y \neq y'$ then we can swap elements in pairs and reduce $(1, 2)$ or $(a, 1)$. Hence we may assume that $R$ contains $(1, x), (x, 2), (y, 1)$ and $(a, y)$. Now by Remark 5.1 we have $(y, 1) = (2, 1)$, so we can reduce $(1, 2)$ after applying the cubic relation

$$(1, x) + (x, 2) + (2, 1) = (1, 2) + (2, x) + (x, 1).$$

6. Only two different indices in pairs

Assume that $(1, 2) \in L$ and $L$ contains only pairs $(1, 2)$ or $(2, 1)$ (where the second type does not have to appear at all). Moreover, in $R$ also at most two indices appear in pairs. Thus if $R$ contains pairs $(1, x)$ and $(y, 2)$ then we have an immediate reduction $(x = 2, y = 1)$. By Lemma 2.2 we are left with two cases, depending on which component of $(1, 2)$ appears in $R$ just in a triple. They are symmetric, hence we consider just one of them.
Assume that \((1, x) \in R\) and \((2, s, t) g_2 \in R\). Then if \(x \notin \{s, t\}\), we can use the relation \((2, s, t) g_2 + (1, x) = (x, s, t) g_2 + (1, 2)\) and reduce \((1, 2)\). Hence we may assume that if \(2\) appears with \(g_2\) in \(R\) then it is always in a triple with \(x\).

Then \(x\) appears with \(g_2\) in \(L\). It cannot be in a pair, because \(x \notin \{1, 2\}\). If there is a triple \((x, c, d) g_2\) such that \(2 \notin \{c, d\}\) then we can use the relation \((x, c, d) g_2 + (1, 2) = (2, c, d) g_2 + (1, x)\) and reduce \((1, x)\). Hence we may assume that \(x\) appears with \(g_2\) in \(L\) only in triples containing \(2\) and we apply Lemma 3.1 applied to occurrences of \(2\) and \(x\) with \(g_2\). This case finishes the whole proof.

References

[BW07] W. Buczyńska and J. A. Wiśniewski, On geometry of binary symmetric models of phylogenetic trees, J. Eur. Math. Soc. 9(3) (2007), 609–635.

[CFSM14] M. Casanellas, J. Fernández-Sánchez, and M. Michałek, Local description of phylogenetic group-based models, arXiv:1402.6945 [math.AG] (2014).

[CLS11] D. Cox, J. Little, and H. Schenck, Toric varieties, Graduate Studies in Mathematics, vol. 124, American Mathematical Society, 2011.

[DBM12] M. Donten-Bury and M. Michałek, Phylogenetic invariants for group based models, Journal of Algebraic Statistics 3 (2012), no. 1, 44–63.

[DE12] J. Draisma and R. H. Eggermont, Finiteness results for abelian tree models, to appear in J. Eur. Math. Soc. (2012).

[DK09] J. Draisma and J. Kuttler, On the ideals of equivariant tree models, Mathematische Annalen 344(3) (2009), 619–644.

[LM14] M. Lasoń and M. Michałek, On the toric ideal of a matroid, Advances in Mathematics 259 (2014), 1–12.

[Man09] C. Manon, The algebra of Conformal Blocks, preprint at arXiv:0910.0577 (2009).

[Mic11] M. Michałek, Geometry of phylogenetic group-based models, Journal of Algebra 339 (2011), 339–356.

[Mic13] ______, Constructive degree bounds for group-based models, Journal of Combinatorial Theory A 120(7) (2013), 1672–1694.

[SS03] C. Semple and M. Steel, Phylogenetics, Oxford University Press, 2003.

[SS05] B. Sturmfels and S. Sullivant, Toric ideals of phylogenetic invariants, J. Comput. Biology 12 (2005), 204–228.

[SSE93] L. A. Székely, M. A. Steel, and P. L. Erdős, Fourier calculus on evolutionary trees, Appl. Math. 14(2) (1993), 200–210.

[Stu96] B. Sturmfels, Groebner bases and convex polytopes, University Lecture Series, vol. 8, American Mathematical Society, 1996.

[Sul07] S. Sullivant, Toric fiber products, J. Algebra 316 (2007), 560–577.