RELEVANT PHYLOGENETIC INVARIANTS OF EVOLUTIONARY MODELS

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ABSTRACT. Recently there have been several attempts to provide a whole set of generators of the ideal of the algebraic variety associated to a phylogenetic tree evolving under an algebraic model. These algebraic varieties have been proven to be useful in phylogenetics. In this paper we prove that, for phylogenetic reconstruction purposes, it is enough to consider generators coming from the edges of the tree, the so-called edge invariants. This is the algebraic analogous to Bunean’s Splits Equivalence Theorem. The interest of this result relies on its potential applications in phylogenetics for the widely used evolutionary models such as Jukes-Cantor, Kimura 2 and 3 parameters, and General Markov models.

1. Introduction

Algebraic evolutionary models and the algebraic varieties associated to a tree evolving under these models have been an interdisciplinary area of research with successful results in the last five years. The use of polynomials in phylogenetic reconstruction was first introduced by biologists Cavender and Felsenstein [CF87] and Lake [Lak87]. Because of their interest in phylogenetics, there have been several attempts to provide a set of generators of the ideal of these algebraic varieties (see for example [AR07], [SS05], [DK09], [CS05]). On the other hand, the authors of this paper have proven in [CFS07] that these generators can be successfully used in phylogenetic reconstruction. In other words, methods based in algebraic geometry can lead to the inference of the phylogenetic tree of current biological species. As we already did in [CF08], our aim in the present paper is to address again the study of these algebraic varieties towards their real applications in phylogenetics.

Algebraic evolutionary models include the algebraic version of widely used models in biology such as Jukes-Cantor model [JC69], Kimura 2 and 3 parameters model (cf. [Kim80], [Kim81]) and the general Markov model (cf. [BH87]). These models belong to what Draisma and Kuttler call equivariant models in [DK09] (see section 2 for the precise definition). Following ideas of Allman and Rhodes and using representation theory, Draisma and Kuttler have recently given an algorithm to obtain the generators of the ideal of the algebraic varieties associated to a tree of $n$ species evolving under an equivariant model from the generators of the ideal associated to
a tree of 3 species and certain minors of matrices (the so-called \textit{edge invariants}). Nevertheless, a set of generators for trees of 3 species is not known for certain models such as the general Markov model (this is the so-called Salmon Conjecture) or the strand symmetric model (see [CS05]). Therefore, a complete list of generators for a tree of \( n \) species evolving under these models cannot be given at this point.

The goal of this paper is to prove that, whereas mathematically speaking it is interesting to know a set of generators of the ideal of these varieties, for biological purposes it is enough to consider certain generators. More precisely, the edge invariants mentioned above suffice to reconstruct the phylogenetic tree of any number of species (see the Theorem in the next page or Theorem 4.4). This is a natural result if one thinks of the combinatorics result of Buneman that says that a tree can be recovered if one knows the set of splits on the set of leaves induced by its edges (cf. [Bun71], [PS05 Theorem 2.35], see also Theorem 4.1 below).

Our inspiration goes back to the work [Fel91] of biologist Joe Felsenstein who calls \textit{phylogenetic invariants} to those polynomial expressions that vanish on the expected frequencies of any sequences arising from one tree topology but are non zero for at least one tree of another topology. A tree topology in this setting is the topology of the tree graph labelled at the leaves with the name of the species. Algebraically speaking, he calls \textit{phylogenetic invariants} to those elements of the ideal associated to a phylogenetic tree that allow to distinguish it from other tree topologies. In the mathematical context, the name phylogenetic invariants has usually been given to all elements of the ideal, see for instance the work of Allman and Rhodes [AR07].

We want to go back to the original meaning of phylogenetic invariants because our focus is devoted to the applications of algebraic geometry in the reconstruction of the tree topology of current species. Therefore, we are mainly interested in precisely those elements of the ideal that provide information for phylogenetic reconstruction purposes; in other words, we are interested in \textit{phylogenetic} invariants (i.e polynomials in the ideal of one tree topology of \( n \) species but not in the ideal of all other tree topologies on the same number of species) and the word \textit{invariants} alone shall mean any element of the ideal. In colloquial language the main result of this paper is that, for phylogenetic reconstruction purposes, the relevant phylogenetic invariants are the edge invariants mentioned above.

As our aim is to study these varieties regarding their applications in biology, let us roughly explain here how does algebraic geometry interfere with phylogenetic reconstruction. Let \( n \) be a number of biological species and assume that we are given an alignment of DNA sequences corresponding to them (the definition of alignment is rather technical but it refers to a collection of \( n \)-tuples in \( \{A,C,G,T\}^n \) that will be also called columns of the alignment). Each column stands for sites in the \( n \) DNA sequences that have evolved from the same nucleotide in the common ancestor. We assume that these species are leaves of a phylogenetic tree \( T \) evolving under a probabilistic model \( \mathcal{M} \) (in this paper we will only consider equivariant models, see Definition 2.4 for the precise definition). It is usual to assume as well that all
columns of the alignment behave independently and identically (i.e. all sites of the DNA sequences of these species evolve in the same way and independently of the other sites). Associated to this model $\mathcal{M}$ there is a parameterization map $\Psi_T$ giving the joint distribution of states $A, C, G, T$ at the leaves of $T$ as polynomial functions of continuous parameters. Therefore, as an alignment of DNA sequences evolving under this model on a tree $T$ is a collection of observations of states at the leaves, it corresponds to a point in the image of this parameterization map. The algebraic variety $V_\mathcal{M}(T)$ associated to $T$ is the closure of this image (see Definition 2.7). In the real life, alignments are not points of $V_\mathcal{M}(T)$ but they are close to $V_\mathcal{M}(T)$ if the model reasonably fits the data. Therefore the idea behind phylogenetic algebraic geometry is to use the ideal of $V_\mathcal{M}(T)$ in order to infer the tree topology $T$. See [CGS05] for an algorithm of phylogenetic reconstruction based on the generators of this ideal and [CFS07] for tests of it on simulated data.

Up to now, all attempts have focused on giving a whole set of generators of $I(V_\mathcal{M}(T))$ but our approach is more practical. As biologists assume that the model $\mathcal{M}$ fits the data, the point given by an alignment is therefore assumed to be close to the union of all varieties $V_\mathcal{M}(T)$ for trees of $n$ species evolving under model $\mathcal{M}$. Henceforth, we only need to know how is a particular variety $V_\mathcal{M}(T_0)$ defined inside $\cup_T V_\mathcal{M}(T)$ where the union runs over all trivalent tree topologies $T$ of $n$ species. In this algebraic geometry context our main result (Theorem 4.4) can be summarized in the following way.

**Theorem.** Let $\mathcal{T}$ be the set of trivalent tree topologies on $n$ leaves and let $\mathcal{M}$ be an equivariant model. For each tree topology $T \in \mathcal{T}$ there exists an open set $U_T$ such that if $p$ belongs to $\cup_{T \in \mathcal{T}} U_T$, then $p$ belongs to a particular variety $V_\mathcal{M}(T_0)$ if and only if $p$ belongs to the zero set of edge invariants of $T_0$.

This result has also other consequences in phylogenetics. For instance, it says that edge invariants should not be used for model fitting tests (see [GP04] for an algebraic introduction to the subject) or for the study of identifiability of continuous parameters (see [AR08] for an explanation of these terminology) of the model because they are indeed phylogenetic invariants. Instead, they should be used in discussing the identifiability of tree topology of such models (see Corollary 3.9) as it was already done by Allman and Rhodes in [AR06]. We also find invariants (not phylogenetic invariants) that could potentially be used for model fitting tests, that is, linear polynomials that can be used for choosing the evolutionary model that best fits the data (see Remark 2.8).

Moreover, our main theorem allows one to give the exact degrees of those generators relevant in phylogenetics (see Corollary 4.12), whereas the degrees of a whole set of generators for the general Markov or strand symmetric models are still unknown. It is worth highlighting that these degrees can be computed by just knowing the model we are interested in, and they do not depend on the topology or the number of leaves we are considering.
Here we outline the structure of the paper. In section 2 we adapt the setting and notation of [DK09] to our convenience. As well, we prove and recall basic facts of group representation theory for those non-familiarized readers. Section 3 is devoted to prove a technical result that will be the key in the proof of our main theorem. Roughly speaking this result proves that edge invariants are indeed phylogenetic invariants for any equivariant model. This was already known for the general Markov model by Allman, Rhodes (see for instance [AR06]) and Eriksson [Eri05] but it is new for the remaining equivariant models. The proof relies on providing a formula for the rank of the flattening of the tensor $\Psi_T$ along any bipartition of the set of leaves. In section 4 we prove Theorem 4.4 our main result. In the last section we provide an exhaustive collection of examples on how to compute the required edge invariants for the most used evolutionary models: Jukes-Cantor, Kimura 2 and 3 parameters, strand symmetric and general Markov model. We compute them explicitly for quartet trees. It is our aim to make this section clear enough for biomathematicians so that, for example, we relate invariants used by biologist like Lake (see [Lak87]) to the more technical definition of edge invariants (see the end of subsection 5.5). We also connect our edge invariants to Fourier coordinates that are more familiar to those readers used to group-based models. In particular, the reader can visualize what are the Fourier coordinates that are actually interesting in biology as not all of them are needed for phylogenetic reconstruction. This section is also a useful illustration of technical definitions given in sections 2 and 3 so it is a good idea to combine the reading of both sections with section 5.

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2. Preliminaries

A tree is a connected finite graph without cycles, consisting of vertices and edges. Given a tree $T$, we write $V(T)$ and $E(T)$ for the set of vertices and edges of $T$. The degree of a vertex is the number of edges incident on it. The set $V(T)$ splits into the set of leaves $L(T)$ (vertices of degree one) and the set of interior vertices $\text{Int}(T)$: $V(T) = L(T) \cup \text{Int}(T)$. One says that a tree is trivalent if each vertex in $\text{Int}(T)$ has degree 3. A tree topology is the topological class of a tree where every leaf has been labelled. Given a subset $L$ of $L(T)$, the subtree induced by $L$ is just the smallest tree composed of the edges and vertices of $T$ in any path connecting two leaves in $L$.

Given an ordered set $B = \{b_1, b_2, \ldots, b_k\}$, we define $W = \langle B \rangle_C$ as the $\mathbb{C}$-vector space generated by the elements of $B$. For biological applications, the most common values of $k$ are 2, 4 or 20 (for example, $B = \{A, C, G, T\}$). Now, given a subgroup $G$ of the group $\mathfrak{S}_k$ of permutations of $k$ elements, we consider the restriction to $G$ of the natural linear representation

$$\rho : \mathfrak{S}_k \rightarrow GL(W)$$
given by the permutation of the elements of $B$. This representation induces a $G$-module structure on $W$ by taking

$$g \cdot u := \rho(g)(u) \in W.$$ 

In fact, $\rho$ induces a $G$-module structure on any tensor power of $W$, say $\otimes^l W := W \otimes \ldots \otimes W$, by taking

$$(2.1) \quad g \cdot (u_1 \otimes \ldots \otimes u_l) := g \cdot u_1 \otimes \ldots \otimes g \cdot u_l.$$ 

Henceforth, any tensor power of $W$ will be implicitly considered as a $G$-module with this action.

From now on, we fix an ordered set $B = \{b_1, b_2, \ldots, b_k\}$, $W = \langle B \rangle_\mathbb{C}$ and a subgroup $G \subset S_k$ acting on $W$ as above.

**Definition 2.1.** A phylogenetic tree on $(G, W)$ is a tree where every vertex $p$ has a $\mathbb{C}$-vector space $W_p \cong W$ associated to it, regarded as a representation of $G$ via the map $\rho$ defined above.

**Notation.** The scalar product with orthonormal basis $B_p$ will be denoted by $(.|.)_p$. This gives a canonical isomorphism from $W_p$ to $W_p^*$. Notice that the scalar product $(.|.)_p$ is $G$-invariant, that is, $(g\cdot u | g\cdot v)_p = (u | v)_p$ for every $u, v \in W_p$ and any $g \in G$.

**Definition 2.2.** Given a phylogenetic tree $T$ on $(G, W)$, a $T$-tensor is any element of

$$\mathcal{L}(T) := \otimes_{p \in \mathcal{L}(T)} W_p.$$ 

A $G$-tensor on $T$ is a $T$-tensor invariant by the action defined in (2.1). The set of $G$-tensors will be denoted by $\mathcal{L}(T)^G$.

From now on, if $l > 0$ we write $\otimes^l W = W \otimes \ldots \otimes W$. We denote by $B(\otimes^l W)$ the basis of $\otimes^l W$ given by

$$\{u_{i_1} \otimes \ldots \otimes u_{i_l} | u_{i_j} \in B\}.$$ 

This is an orthonormal basis with respect to the scalar product of $\otimes^l W$ given by

$$(\otimes_p u_p | \otimes_p v_p) = \prod_p(u_p | v_p).$$ 

If $L \subset \mathcal{L}(T)$ is a subset of $\mathcal{L}(T)$ and $l = \#L$, then we shall use the notation $\otimes_L W$ for the space $\otimes_{p \in \mathcal{L}} W_p \cong \otimes^l W$.

**Definition 2.3.** Let $T$ be a phylogenetic tree on $(G, W)$ and assume that a distinguished vertex of $T$ (the root) is given, inducing an orientation in all the edges of $T$: write $e_0$ and $e_1$ for the origin and final vertices of the edge $e$, respectively. A $G$-evolutionary presentation\(^1\) of $T$ is a collection of tensors $\{A_{e_0,e_1}\}_{e \in E(T)}$ where each $A_{e_0,e_1}$ is a $G$-invariant element of the $G$-module $W_{e_0} \otimes W_{e_1}$. The space of $G$-invariant elements of $W_{e_0} \otimes W_{e_1}$ is denoted by $(W_{e_0} \otimes W_{e_1})^G$.

\(^1\)Notice that evolutionary presentations are called representations in [DK09]. We prefer this terminology to avoid confusion with representation theory.
If another root (orientation) on $T$ is considered, inducing the opposite orientation on some edge $e \in E(T)$, we define $A_{e_1,e_0} := A_{e_0,e_1}$, where $t$ is the natural isomorphism $(W_{e_0} \otimes W_{e_1})^G \cong (W_{e_1} \otimes W_{e_0})^G$. We will often identify $\text{Hom}_G(W_{e_0}, W_{e_1})$ with $(W_{e_0} \otimes W_{e_1})^G$ via $W_{e_0}^* \cong W_{e_0}$. With this convention, $G$-evolutionary presentations on a tree do not depend on the orientation chosen. The space of all $G$-evolutionary presentations of $T$ is the parameter space denoted by $\text{Par}_G(T) = \prod_{e \in E(T)} (W_{e_0} \otimes W_{e_1})^G$. Notice that a $G$-evolutionary presentation of $T$ induces by restriction a $G$-evolutionary presentation of any subtree of $T$.

The space $\text{Par}_G(T)$, as well as $L(T)$ and $L(T)^G$, are irreducible affine spaces with their Zariski topology.

**Definition 2.4.** An equivariant model of evolution is a pair $(G, W)$ as above, $W = \langle b_1, \ldots, b_k \rangle$, $G \subset \mathfrak{S}_k$. Trees evolving under this equivariant model are phylogenetic trees on $(G, W)$ together with the space of $G$-evolutionary presentations.

Equivariant models of evolution include the general Markov model [BH87] when $G = \{\text{id}\}$, the strand symmetric model [CS05] when $G = \langle (AT)(CG) \rangle$, and the algebraic versions of Kimura 3-parameters [Kim81] ($G = \langle (AC)(GT), (AG)(CT) \rangle$), Kimura 2-parameters [Kim80] ($G = \langle (ACGT), (AG) \rangle$) and Jukes-Cantor models [JC69] ($G = \mathfrak{S}_4$). We derive the reader to section 5 for specific computations with these models.

Following [AR07] and [DK09] we present now a fundamental operation $*$ on phylogenetic trees, $G$-evolutionary presentations and $T$-tensors. To this aim, we first introduce a bilinear operation $\langle \cdot | \cdot \rangle$ between tensors induced by the bilinear form $(\cdot | \cdot)$ on $W$. Let $X$ and $Y$ be two finite sets of indices with $Z = X \cap Y \neq \emptyset$, and such that every $p$ in $X$ or $Y$ has associated a vector space $W_p \cong W$ to it. Define

$$\langle \cdot | \cdot \rangle : \otimes_X W \times \otimes_Y W \rightarrow \otimes_{X \cup Y \setminus Z} W$$

$$(\otimes_{p \in X} v_p, \otimes_{p \in Y} u_p) \mapsto \left( \otimes_{p \in Z} v_p, \otimes_{p \in Z} u_p \right) \left( \left( \otimes_{p \in X \setminus Z} v_p \right) \otimes \left( \otimes_{p \in Y \setminus Z} u_p \right) \right)$$

Now, we define the $*$ operation:

* **for trees:** Given $l$ spaced trees $T_1, \ldots, T_l$ whose vertex sets only share a common leaf $q$ with common space $W_q$ and common basis $B_q$, we construct a new spaced tree $*T_i$ obtained by gluing the $T_i$’s along $q$; the space at a vertex of $*T_i$ coming from $T_j$ is just the space attached to it in $T_j$, with the same distinguished basis.

* **for $G$-evolutionary presentations:** Given $G$-evolutionary presentations $A_i \in \text{Par}(T_i)$ for $i = 1, \ldots, l$, we denote by $*A_i$ the $G$-evolutionary presentation of $*T_i$ built up from the $A_i$.

* **for tensors:** Now let $\psi_i$ be a $T_i$-tensor, for all $i$. Then we obtain a $T$-tensor as follows:

$$*T_i \psi_i := \sum_{b \in B_q} \otimes_i \langle b | \psi_i \rangle.$$

Although this $*$ operator is not a binary operator extended to several factors, when convenient we will write $T_1 \ast \ldots \ast T_l$ for $*T_i$ and $\psi_1 \ast \ldots \ast \psi_l$ for $*\psi_i$. 

Notation 2.5. A slightly more general $\ast$-operation will be needed in forthcoming section 3. Given $\varphi_A \in (\otimes_X W)^G$ and $\varphi_2 \in (\otimes_Y W)^G$, define

$$\varphi_1 \ast \varphi_2 = \sum_{b \in B(\otimes_Z W)} \langle \varphi_1 | b \rangle \otimes \langle \varphi_2 | b \rangle \in (\otimes_{X \cup Y \setminus Z} W)^G.$$  

Clearly, if $T_1$ and $T_2$ are two phylogenetic trees that share a common leaf $q$, then this definition agrees with the $\ast$-operation defined above.

Now we describe a basic procedure that allows us to associate a $T$-tensor to any $G$-evolutionary presentation of $T$. We proceed inductively on the number of edges to define $\Psi_T : \mathrm{Par}(T) \to \mathcal{L}(T)$. Let $A \in \mathrm{Par}(T)$. First, if $T$ has a single edge $p, q$, then $\Psi_T(A) := A_{qp}$, is an element of $\mathcal{L}(T) = W_q \otimes W_p$. If $T$ has more than one edge, then let $q$ be any internal vertex of $T$. Two vertices $p, q \in T$ are adjacent if they are joined by an edge; in this case, we write $p \sim q$. We can then write $T = \ast_{p \sim q} T_p$, where $T_p$ is the branch of $T$ around $q$ containing $p$, constructed by taking the connected component of $T \setminus \{q\}$ containing $p$, and reattaching $q$ to $p$. The $G$-evolutionary presentation $A$ induces $G$-evolutionary presentations $A_p$ of the $T_p$, and by induction $\Psi_{T_p}(A_p)$ has been defined. We now set

$$\Psi_T(A) := \ast_{p \sim q} \Psi_{T_p}(A_p).$$

This definition is independent of the choice of $q$ and the formula is also valid if $q$ is actually a leaf (see [DK09] for details). Moreover, we have that the map $\Psi_T : \mathrm{Par}_G(T) \to \mathcal{L}(T)$ is $G$-equivariant (see [DK09, Lemma 5.1]).

Remark 2.6. Notice that the above map $\Psi_T : \mathrm{Par}_G(T) \to \mathcal{L}(T)^G$ is a continuous map in the Zariski topology.

Definition 2.7. The algebraic variety associated to a phylogenetic tree $T$ on $(G, W)$ is

$$V_G(T) := \overline{\{\Psi_T(A) \mid A \in \mathrm{Par}_G(T)\}} \subset \mathcal{L}(T)$$

where the closure is taken in the Zariski topology.

Notice that we have $V_G(T) \subset \mathcal{L}(T)^G$. From now on, we will consider $\mathcal{L}(T)^G$ as the ambient space of $V_G(T)$ and $\mathcal{I}(T)$ will be the ideal of this variety in the corresponding coordinate ring. When the group is understood from the context, we will use the notation $V(T)$.

Remark 2.8. The inclusion $\mathcal{L}(T)^G \subseteq \mathcal{L}(T)$ is defined by a set of linear polynomials that are also invariants of any phylogenetic tree $T$ on $(G, W)$ (see the Introduction for the explanation of the word invariants). Although they are not phylogenetic invariants because they vanish on $V_G(T)$ for any tree $T$, they might be interesting for choosing the model $(G, W)$ that best fits the data. This application of invariants to model fitting will be studied in a forthcoming paper.
Example 2.9. If we consider \( B = \{ A, C, G, T \} \) and \( G = \{ \text{id} \} \subset \mathcal{G}_4 \), we obtain the general Markov model. In this case, \( (W_{e_0} \otimes W_{e_1})^G = (W_{e_0} \otimes W_{e_1}) \) and no restrictive conditions are imposed on the parameters of the model. Thus, a \( G \)-evolutionary presentation can be identified, by taking the basis \( B \) in \( W \) with a collection of matrices \( \{ A_e \}_{e \in E(T)} \) and the parameters of the model are the entries of these matrices. When these entries are real non-negative values and their columns sum to 1, they can be understood as the probabilities of substitution among the 4 nucleotides:

\[
A_e = \begin{pmatrix}
P(\text{A} \mid \text{A}, e) & P(\text{A} \mid \text{C}, e) & P(\text{A} \mid \text{G}, e) & P(\text{A} \mid \text{T}, e) \\
P(\text{C} \mid \text{A}, e) & P(\text{C} \mid \text{C}, e) & P(\text{C} \mid \text{G}, e) & P(\text{C} \mid \text{T}, e) \\
P(\text{G} \mid \text{A}, e) & P(\text{G} \mid \text{C}, e) & P(\text{G} \mid \text{G}, e) & P(\text{G} \mid \text{T}, e) \\
P(\text{T} \mid \text{A}, e) & P(\text{T} \mid \text{C}, e) & P(\text{T} \mid \text{G}, e) & P(\text{T} \mid \text{T}, e)
\end{pmatrix}.
\]

Here \( P(x \mid y, e) \) is the conditional probability that nucleotide \( Y \) at the parent species \( e_0 \) is being substituted along edge \( e \) by nucleotide \( X \) at its child species \( e_1 \). In our terminology introduced above, \( P(x \mid y, e) \) is the coordinate of \( A_e \in W_{e_0} \otimes W_{e_1} \cong W \otimes W \) corresponding to \( Y \otimes X \). Given a tree \( T \), the \( G \)-equivariant map \( \Psi_T \) is the parameterization that associates to each parameter set the vector of expected pattern frequencies \( p = (p_{x_1x_2...x_n})_{x_1 \in B} \) (that is, \( p_{x_1x_2...x_n} \) is the probability of observing \( x_1x_2...x_n \) at the leaves of \( T \)). For example, if \( T \) is a 4-leaf tree as in figure 1 then

\[
\Psi_T : \prod_{e \in E(T)} (W \otimes W) \cong \mathbb{C}^{80} \rightarrow \otimes^4 W \cong \mathbb{C}^{256}
\]

\[
(A_e)_e \mapsto (p_{\text{AAAA}}, p_{\text{AAAC}}, \ldots, p_{\text{TTTT}})
\]

and \( p_{x_1x_2x_3x_4} \) is the coordinate of \( p \in \mathcal{L}(T) \cong \mathbb{C}^{256} \) corresponding to the basis vector \( x_1 \otimes x_2 \otimes x_3 \otimes x_4 \). In this case, the image of \( \Psi_T \) is given by

\[
p_{x_1x_2x_3x_4} = \sum_{y,z} \pi_Y A_e(y) A_{e(1)}(x_1, y) A_{e(2)}(x_2, y) A_{e(3)}(x_3, z) A_{e(4)}(x_4, z).
\]

Here \( \pi_Y \) is the probability of nucleotide \( Y \) occurring at the root node (see figure 1). Actually, in the original definition of \( \Psi_T \) (see paragraph before Remark 2.6) we gave a reparameterization of \( V_G(T) \) where we omit parameters \( \pi_Y \) for convenience.

Definition 2.10. Given a tree \( T \), a bipartition of the leaves of \( T \) is a decomposition \( L(T) = L_1 \cup L_2 \) where \( L_1 \cup L_2 = \emptyset \). We denote it as \( L_1 \mid L_2 \). Notice that every edge
e of $T$ induces a bipartition $L_1 \mid L_2$ of $L(T)$ by removing it; such a bipartition is called an edge split of $T$ and will be denoted by the same letter $e$.

2.1. **Representation Theory.** We will make use of representation theory of groups. A basic reference for this are the books [Ser77] and [FH91] and the reader is referred to them for definitions and well-known facts.

From now on, write $\Omega_G = \{\omega_1, \ldots, \omega_s\}$ for the set of irreducible characters of $G$. It is known that any two representations with the same character are isomorphic (Corollary 2 of §2 of [Ser77]). As a consequence of this and Schur’s lemma (see §2.2 of [Ser77]) we obtain the following fundamental result in representation theory:

**Lemma 2.11.** Let $N_\omega, N_{\omega'}$ be the irreducible linear representations of $G$ with associated characters $\omega, \omega' \in \Omega_G$. If $f : N_\omega \to N_{\omega'}$ is a $G$-module homomorphism, and

(i) if $\omega \neq \omega'$, then $f = 0$;
(ii) if $\omega = \omega'$, then $f$ is a homothety.

In particular, $\text{Hom}_G(N_\omega, N_\omega) \cong \mathbb{C}$.

For every irreducible character $\omega_t \in \Omega_G$, fix an irreducible $G$-module $N_{\omega_t}$ with associated character $\omega_t$. Then, for any $G$-module $V$, there exists a unique decomposition of $V$ into isotypic components:

$$V \cong \bigoplus_{t=1}^s V[\omega_t]$$

where each $V[\omega_t]$ is isomorphic to $N_{\omega_t} \otimes \mathbb{C}^{m(\omega_t, V)}$ for some multiplicity $m(\omega_t, V)$, $t = 1, \ldots, s$. We also have that if $V'$ is another representation of $G$, then

$$\text{Hom}_G(V, V') \cong \bigoplus_{t=1}^s \text{Hom}_C(\mathbb{C}^{m(\omega_t, V)}, \mathbb{C}^{m(\omega_t, V')})$$

Going back to our fixed vector space $W$, we already know that the space $\otimes^l W$, $l > 0$ is a $G$-representation as well and, as such,

$$\otimes^l W \cong \bigoplus_{t=1}^s N_{\omega_t} \otimes \mathbb{C}^{m(\omega_t, \otimes^l W)}.$$

We will denote by $m(l)$ the $s$-tuple

$$m(l) = (m(\omega_1, \otimes^l W), \ldots, m(\omega_s, \otimes^l W)).$$

In particular, $m(1)$ will be denoted by $m = (m_1, \ldots, m_s)$. Moreover, if $\chi$ denotes the associated character to the representation $\rho : G \to GL(W)$, the decomposition (2.2) above induces an equality of characters

$$\chi = \sum_{t=1}^s m_t \omega_t \quad m_t \in \mathbb{Z}.$$

If $a = (a_t)_{t=1,\ldots,s}, b = (b_t)_{t=1,\ldots,s} \in \mathbb{N}^s$, we write $a \leq b$ if $a_t \leq b_t$ for each $t = 1, \ldots, s$. Similarly, $\min\{a, b\}$ is the $s$-tuple given by the minimum of each entry.

**Lemma 2.12.** With this notation, we have $m(l) \leq m(l')$ if $l \leq l'$. 
Definition 2.14. Let $T$ be a phylogenetic tree on $(G,W)$ and let $L_1 \mid L_2$ be a bipartition of its leaves with $l_1 = \frac{1}{2} L_1$ and $l_2 = \frac{1}{2} L_2$. Let $\psi$ be a $G$-tensor on $T$.

The **flattening of** $\psi$ **along** $L_1 \mid L_2$, denoted by $\text{flat}_{L_1|L_2} \psi$, is the image of $\psi$ via the isomorphism

$$\mathcal{L}(T)^G \cong \text{Hom}_G(\otimes_{L_1} W, \otimes_{L_2} W).$$

The **thin flattening of** $\psi$ **along** $L_1 \mid L_2$ is the $s$-tuple of linear maps, denoted by $Tf_{L_1|L_2}(\psi)$, obtained from $\text{flat}_{L_1|L_2} \psi$ via the isomorphism

$$\text{Hom}_G(\otimes_{L_1} W, \otimes_{L_2} W) \cong \bigoplus_{t=1}^s \text{Hom}_\mathbb{C}(\mathbb{C}^{m(l_1)t}, \mathbb{C}^{m(l_2)t}).$$

Remark 2.15. Notice that the composition of linear maps induce a composition of flattenings and thin flattenings. Notice also that if $\psi \in \mathcal{L}(T)^G$ and $L_1 \mid L_2$ is a bipartition of $L(T)$, then

$$(\text{flat}_{L_1|L_2} \psi)(u) = \langle \psi \mid u \rangle, \quad \forall u \in \otimes_{L_1} W$$

where $\langle \cdot \mid \cdot \rangle$ is the operation defined in (2.2).

Notation 2.16. If $Tf_{L_1|L_2}(\psi) = (\psi_1, \psi_2, \ldots, \psi_s)$, we write

$$\text{rk} \; Tf_{L_1|L_2}(\psi) = (\text{rk} \; (\psi_1), \ldots, \text{rk} \; (\psi_s)).$$

We also denote $\text{rk} \; Tf_{L_1|L_2}(\psi) = \sum_{t=1}^s \text{rk} \; (\psi_t)$ and call it the **rank** of $Tf_{L_1|L_2}(\psi)$. Clearly, this definition is coherent with the usual definition of rank if we regard $Tf_{L_1|L_2}(\psi)$ as a $\mathbb{C}$-linear map $\mathbb{C}^\sum_i m(l_1)i \to \mathbb{C}^\sum_i m(l_2)i$. 

Proof. We prove that $m(l) \leq m(l+1)$ for any $l$. First of all, we show that if $\omega_1 \in \Omega$ is the trivial character, then $m_1 \geq 1$. To this aim, notice that the vector $\sum_{b \in B} b \in W$ is invariant by the action of any $g \in G$. In particular, we have $\sum_{b \in B} b \in W[\omega_1]$ and so $\omega_1$ does appear in the decomposition of $\chi$ with non-zero coefficient. Now, given $l > 0$, write $\chi^l = \sum_t a_t \omega_t$. The claim follows from the fact that the coefficient of any irreducible character of $G$, say $\omega_t$, in $\chi^{l+1}$ is just $m_1 a_t + \ldots \geq a_t$. □
The following easy lemma is left to the reader:

**Lemma 2.17.** We have that $\text{rk} \ flat_{L_1|L_2} \psi = \sum_{t=1}^s \dim_{\mathbb{C}} N_{\omega_t} \text{rk} (\psi_t)$. Moreover, the following are equivalent

(i) $\text{rk} \ flat_{L_1|L_2} \psi$ is maximal;
(ii) $\text{rk} (\psi_t)$ is maximal $\forall t \in \{1, 2, \ldots, s\}$;
(iii) $\text{rk} \ Tf_{L_1|L_2} (\psi)$ is maximal;
(iv) $\text{rk} \ Tf_{L_1|L_2} (\psi)$ is maximal.

**Remark 2.18.** Once a basis for every $C_m(l_i)_{t}$ is chosen, we can identify $\bigoplus_{t=1}^s \text{Hom}_{\mathbb{C}}(C_m(l_1)_{t}, C_m(l_2)_{t})$ with the space of block-diagonal matrices $M_m(l_1)_{m(l_2)}$. The notation introduced is coherent with Notation 2.13.

**Lemma 2.19.** Let $\varphi_1 \in (\otimes_{L_1 \cup C} W)^G$ and $\varphi_2 \in (\otimes_{L_2 \cup C} W)^G$ be two tensors. Then,

(a) $\text{flat}_{L_1|L_2} (\varphi_1 \varphi_2) = \text{flat}_{L_1|C} (\varphi_1) \text{flat}_{C|L_2} (\varphi_2)$;
(b) $\text{Tf}_{L_1|L_2} (\varphi_1 \varphi_2) = \text{Tf}_{L_1|C} (\varphi_1) \text{Tf}_{C|L_2} (\varphi_2)$.

**Notation 2.20.** Given an edge $e$, we denote $1_e = \sum_{b \in B} b \otimes b \in (W_{e_0} \otimes W_{e_1})_G$. Given a phylogenetic tree $T$, we write $1_T = (1_e)_{e \in E(T)}$ and call it the no-mutation presentation of $T$.

2.3. **Degenerated trees and trees with observed interior vertices.** For technical reasons, we admit degenerated trees reduced to just one vertex, which is considered as a leaf. If $T = \bullet_q$ is such a tree, we associate the $\mathbb{C}$-vector space $W$ to $q$, making of $T$ a phylogenetic tree on $(G, W)$. Moreover, we take $\text{Par}_G(T)$ to be composed of the no-mutation presentation, that is,

$$\text{Par}_G(T) = \{1_q\} \quad \text{where} \quad 1_q = \sum_{u \in B} u \otimes u.$$ 

and define $\Psi_T : \text{Par}_G(T) \to \mathcal{L}(T)^G = W$ by mapping $1_q$ to $\sum_{u \in B} u$. The reader can think of such a tree as a two-leaf tree where we only accept the no-mutation presentation between its two leaves. All the above definitions are coherent with this interpretation.

**Definition 2.21.** Let $T$ be a phylogenetic tree on $(G, W)$ and let $q \in \text{Int}(T)$. Then, we can write $T = *_{i=1}^m T_i$, where $T_i$ are subtrees of $T$ sharing the vertex $q$ as a common leaf. Write $T_0$ for the degenerated tree reduced to $q$. The tree $T$ with observed $q$ is defined by

$$T^q = *_{i=0}^m T_i.$$
Notice that, by definition, the leaves of $T^q$ are the leaves of $T$, $L(T^q) = L(T)$, while $\mathcal{L}(T^q) = \mathcal{L}(T) \otimes W$. Define a map
\[
\Psi_T^q : \text{Par}_G(T) \to \mathcal{L}(T^q)
\]
by taking $\Psi_T^q(A) = \Psi_T^0(1^q) \ast \Psi_T^1(A_1) \ast \ldots \ast \Psi_T^m(A_m)$, where $A_i$ is the restriction of the $G$-evolutionary presentation $A$ to the subtree $T_i$.

3. The ideal of an equivariant model

In this section, we essentially prove that edge invariants are indeed phylogenetic invariants (see Introduction). The proof of this result is quite technical as it is valid for any equivariant model.

Given a phylogenetic tree $T$ on $(G,W)$ on $W$ and a bipartition $\beta = L_1 \mid L_2$ of the leaves of $T$, define $T_1$ (resp. $T_2$) as the minimal subtree of $T$ that contains the leaves in $L_1$ (resp. $L_2$). Clearly, we have $V(T) = V(T_1) \cup V(T_2)$. Given two vertices $p,q \in V(T)$, the chain $\text{ch}(q,p)$ is the linear subtree composed of the edges and vertices between $q$ and $p$. Define a binary relationship $\sim_{L_1}$ among the leaves of $L_1$ as follows:
\[
x \sim_{L_1} y \quad \text{if} \quad \text{ch}(x,y) \cap T_2 = \emptyset.
\]
Analogously, a binary relationship $\sim_{L_2}$ can be defined. It is easy to check that both $\sim_{L_1}$ and $\sim_{L_2}$ are equivalence relationships. Write $n_1$ and $n_2$ for the cardinals of the equivalence classes of $\sim_{L_1}$ and $\sim_{L_2}$, respectively. For $i = 1,2$, write $\{L_{i,j}\}_{j=1,\ldots,n_i}$ for the resulting equivalence classes in $L_i$, so that $L_i = \bigcup_{j=1}^{n_i} L_{i,j}$. Notice that if $l_1 = \sharp L_1$ and $l_2 = \sharp L_2$, then $n_1 \leq l_1$ and $n_2 \leq l_2$. From now on, we will denote
\[
M_{\beta,T} = \mathbf{m}(\min\{n_1, n_2\}).
\]

The main goal of this section is to prove the following Proposition, which is a generalization of [Eri05, Theorem 19.5] to equivariant models. Its interest lies in the fact that it translates the topology of a tree into rank conditions of suitable matrices.

**Proposition 3.1.** Let $T$ be a trivalent phylogenetic tree on $(G,W)$ and let $\beta = L_1 \mid L_2$ be a bipartition of $L(T)$ as above. Then, we have
\[
\text{rk} \ Tf_\beta(\psi) \leq M_{\beta,T} \quad \forall \psi \in V(T),
\]
and there exists a non-empty Zariski open set $U_\beta \subset V(T)$ such that the equality holds for every $\psi \in U_\beta$. Moreover,

(i) $\beta$ is an edge split in $T$ if and only if $M_{\beta,T} = m$.
(ii) If $\beta$ is not an edge split in $T$, then $M_{\beta,T} \geq m(2)$.

The existence of the Zariski open subset above where the flattening attains the expected rank cannot be proven by a simple dimension counting as the following example shows.
Example 3.2. Consider \( G = \{\text{id}\} \subset \mathcal{G}_4 \) and the quartet tree \( T \) having an inner edge \( e \). Then \( T f_\beta(\psi) \) can be seen as a \( 16 \times 16 \) matrix \( M \) and its expected rank is 4 according to Proposition 3.1(i). The variety \( V_G(T) \) has dimension 60 and is contained in the determinantal variety defined by the \( 5 \times 5 \) minors of \( M \), which has dimension \( 256 - (16 - 5 + 1)(16 - 5 + 1) = 112 \). A priori \( V_G(T) \) could also be included in the variety of \( 4 \times 4 \) minors of \( M \) which has dimension \( 256 - (16 - 4 + 1)(16 - 4 + 1) = 87 \), so that a general element of \( V_G(T) \) would not have the expected rank 4.

Before proving Proposition 3.1 we need to state a couple of lemmas.

**Lemma 3.3.** Let \( T \) be a phylogenetic tree on \( (G, W) \) and let \( \beta = L_1 \mid L_2 \) be a bipartition of \( L(T) \) such that every cherry of \( T \) is composed of one leaf in \( L_1 \) and one leaf in \( L_2 \). For a generic \( G \)-evolutionary presentation \( A \) of \( T \), it holds that \( \text{rk} \ T f_\beta(\Psi_T(A)) = m_{\beta,T} \).

**Proof.** Write \( L_1 = \{u_1, u_2, \ldots, u_{l_1}\} \) and \( L_2 = \{v_1, v_2, \ldots, v_{l_2}\} \), and write \( n = l_1 + l_2 \) for the number of leaves of \( T \). Assume that \( 1 \leq l_1 \leq l_2 \). Notice that with our assumption, we have \( n_1 = l_1, n_2 = l_2 \) and so, \( m_{\beta,T} = m(l_1) \). To reach the claim, we first show that the above condition for the rank \( \text{rk} \) defined an open set in \( \text{Par}_G(T) \). Then, we will prove recursively that this open set is not empty.

Let \( \varphi \in \mathcal{L}(T)^G \) and write \( T f_\beta(\varphi) = (\varphi_1, \varphi_2, \ldots, \varphi_s) \). Then \( T f_\beta(\varphi) \) has maximal rank if and only if

\[
\text{rk} \ \varphi_t = \min\{m(n_1)_t, m(n_2)_t\} \quad \text{for every } t = 1, \ldots, s.
\]

Each rank condition \( \text{rk} \ \varphi_t < \min\{m(n_1)_t, m(n_2)_t\}, t = 1, \ldots, s \) defines a closed proper subset \( Z_t \) of \( \text{Hom}_G(\otimes_{L_1} W, \otimes_{L_2} W) \cong \mathcal{L}(T)^G \). Thus,

\[
\tilde{V} = \mathcal{L}(T)^G \setminus \cup_{t=1}^s Z_t
\]

is a dense open subset in \( \mathcal{L}(T)^G \), and for every \( \varphi \in \tilde{V} \),

\[
\text{rk} \ T f_\beta(\varphi) = m_{\beta,T}.
\]

Moreover, \( \Psi_T : \text{Par}_G(T) \to \mathcal{L}(T)^G \) is a continuous map, so \( V = \Psi_T^{-1}(\tilde{V}) \) is an open set in \( \text{Par}_G(T) \). To prove that \( V \) is non-empty, we will recursively construct a \( G \)-evolutionary presentation \( A \in \text{Par}_G(T) \) with \( A_e = 1_e \) for any terminal edge \( e \), and such that

\[
\text{rk} \ \text{flat}_{L_1 \mid L_2} \Psi_T(A) = k^1.
\]

This implies that the rank of \( \text{flat}_{L_1 \mid L_2} \Psi_T(A) \) is maximal and, by applying (2.17), we derive that so is \( \text{rk} \ T f_\beta(\Psi_T(A)) \). From this, we derive that \( \text{rk} \ T f_\beta(\Psi_T(A)) = m(l_1) = m_{\beta,T} \).

For \( n = 2 \), it is enough to take \( A \) equal to the no-mutation presentation: \( 1_T = \sum_b b \otimes b \). For general \( n \), take a cherry of \( T \). By reordering the leaves of \( L_1 \) and \( L_2 \) if necessary, we can assume that the leaves in this cherry are \( u_{l_1}, v_{l_2} \). Let \( e \) be the edge of \( T \) adjacent to it and insert two vertices \( q_1 \) and \( q_2 \) in the edge \( e \). We obtain
a decomposition of \( T \) as follows: \( T = T^1 \ast T^e \ast T^2 \), where \( T^e \) is a 2-leaf tree with leaves \( q_1 \) and \( q_2 \), and \( T^1 \) and \( T^2 \) are the subtrees of \( T \) obtained when removing \( T^e \) from \( T \) as shown in figure [2]. Then, we have

\[
L(T^1) = \{u_1, u_2, \ldots, u_{l_1-1}, q_1, v_1, \ldots, v_{l_2-1}\},
\]
\[
L(T^e) = \{q_1, q_2\},
\]
\[
L(T^2) = \{u_{l_1}, v_{l_2}, q\}.
\]

Write \( L^{(1)}_1 = \{u_1, \ldots, u_{l_1-1}, q_1\} \) and \( L^{(1)}_2 = \{v_1, \ldots, v_{l_2-1}\} \). Since \( T^1 \) has \( n-1 \) leaves, our assumption says that there is some \( G \)-evolutionary presentation, say \( A_1 \in \text{Par}_G(T^1) \), such that

\[
\text{rk flat}_{L^{(1)}_1 \cup L^{(1)}_2} \Psi_{T^1}(A) = k_{\min(l_1, l_2-1)}.
\]

Define \( A = A^1 \ast A_e \ast 1_{T^2} \in \text{Par}_G(T) \), where \( A_e \in \text{Hom}_G(W_{q_1}, W_{q_2}) \) is generic and we will show that the equality (3.2) holds. To this aim, we claim that

\[
(3.3) \quad \Psi_T(A) = (\Psi_{T^1}(A^1) \otimes 1) \ast L^{(1)}_{1 \cup (q)} \phi(A_e).
\]

**Proof.** First of all, the decomposition \( A = A^1 \ast A_e \ast 1_{T^2} \) induces a decomposition of \( \Psi_T(A) \) as

\[
\Psi_T(A) = \Psi_{T^1}(A^1) \ast \Psi_{T^e}(A_e) \ast \Psi_{T^2}(1_{T^2}) =
\]
\[
= \sum_{z_1, z_2 \in B} (A_e \mid z_1 \otimes z_2) \langle \Psi_{T^1}(A^1) \mid z_1 \rangle \otimes \langle \Psi_{T^2}(1_{T^2}) \mid z_2 \rangle.
\]

and notice that

\[
\langle \Psi_{T^1}(A^1) \mid z_1 \rangle \otimes \langle \Psi_{T^2}(1_{T^2}) \mid z_2 \rangle = \langle \Psi_{T^1}(A^1) \mid z_1 \rangle \otimes (z_2 \otimes z_2) =
\]
\[
= \sum_{b_i \in B} (\Psi_{T^1}(A^1) \mid b_i \otimes \ldots \otimes b_{l_1-1} \otimes z_1) \otimes (z_2 \otimes z_2) \otimes b_1 \otimes \ldots \otimes b_{l_1-1}.
\]
Thus, we obtain that $\Psi_T(A)$ is equal to

$$\sum_{z_1, z_2, b_1, \ldots, b_{l_1-1}} (A_e \mid z_1 \otimes z_2) \langle \Psi_T(A^1) \mid b_1 \otimes \ldots \otimes b_{l_1-1} \otimes z_1 \rangle \otimes z_2 \otimes b_1 \otimes \ldots \otimes b_{l_1-1}. $$

On the other hand, consider the $G$-equivariant map

$$\varphi(A_e) : \otimes_{L_1 \cup \{q_1\}} W \rightarrow \otimes L_1 W$$

$$b_1 \otimes \ldots \otimes b_{l_1-1} \otimes b_1 \otimes b_{q_1} \mapsto (A_e \mid b_1 \otimes b_{q_1}) b_1 \otimes \ldots \otimes b_{l_1-1} \otimes b_{q_1}.$$ 

and define the tensor $\phi(A_e)$ as the image of $\varphi(A_e)$ via the isomorphism

$$\text{Hom}_G(\otimes_{L_1 \cup \{q_1\}} W, \otimes L_1 W) \cong \left((\otimes_{L_1 \cup \{q_1\}} W) \otimes (\otimes L_1 W)\right)^G.$$ 

Thus, if $b_i \in B_{u_i}, i = 1, \ldots, l_1 - 1, z_1 \in B_{q_1}$ and $z_2 \in B_{l_1}$, then

$$\langle \phi(A_e) \mid b_1 \otimes \ldots \otimes b_{l_1-1} \otimes z_1 \otimes z_2 \rangle = (A_e \mid z_1 \otimes z_2) z_2 \otimes b_1 \otimes \ldots \otimes b_{l_1-1}. $$

If $1 = \sum b b \otimes b \in W_{u_1} \otimes W_{u_2}$, we have $\langle 1 \mid z_2 \rangle = z_2$ and so

$$\langle \Psi_T(A^1) \otimes 1 \mid b_1 \otimes \ldots \otimes b_{l_1-1} \otimes z_1 \otimes z_2 \rangle = \langle \Psi_T(A^1) \mid b_1 \otimes \ldots \otimes b_{l_1-1} \otimes z_1 \rangle \otimes z_2.$$ 

Putting all together, we obtain that $(\Psi_T(A^1) \otimes 1) * \phi(A_e)$ is equal to

$$\sum_{b_1, \ldots, b_{l_1-1}, z_1, z_2} (A_e \mid z_1 \otimes z_2) \langle \Psi_T(A^1) \mid b_1 \otimes \ldots \otimes b_{l_1-1} \otimes z_1 \rangle \otimes z_2 \otimes (z_2 \otimes b_1 \otimes \ldots \otimes b_{l_1-1}). $$

This proves the claim.

Now, apply Lemma 2.19 to (3.3) to get

$$\text{flat}_{L_1 \cup L_2} \Psi_T(A) = \text{flat}_{L_1 \cup L_1 \cup \{q\}} (\Psi_T(A^1) \otimes 1) \text{flat}_{L_1 \cup \{q\}} L_2 \phi(A_e).$$ 

It is straightforward to check that

$$\text{flat}_{L_1 \cup \{q\}} L_2 (\Psi_T(A^1) \otimes 1) = \left(\text{flat}_{L_1 \cup \{q\}} L_2 \Psi_T(A^1)\right) \otimes \left(\text{flat}_{\{u_1\}} L_2 \otimes \{v_2\}\right),$$

so the rank of $F := \text{flat}_{L_1 \cup \{q\}} L_2 (\Psi_T(A^1) \otimes 1)$ is equal to the product of ranks: $k \times k^{\min\{l_1-1, l_2\}} = k^{\min\{l_1, l_2+1\}}$. On the other hand, write $G(A_e)$ for the matrix of $\phi(A_e)$ in the basis $B(\otimes L_1 W)$ and $B(\otimes L_1 \cup \{q\} W)$. It is a block diagonal matrix, each block being a convenient column of the matrix $A_e$. Then the rank of $\text{flat}_{L_1 \cup L_2} \Psi_T(A)$ is $k^{l_1}$ if and only if $\text{Ker}(F) \cap \text{Im}(G(A_e)) = \{0\}$. Since this holds for a generic matrix $A_e$, the claim follows. □

**Lemma 3.4.** Let $T$ be a phylogenetic tree on $(G, W)$ and let $q \in \text{Int}(T)$. Assume that $q$ has degree two while the remaining interior vertices have degree three and write $T^q$ for the tree with observed $q$. Then, for a generic $G$-evolutionary presentation $A \in \text{Par}_G(T)$, we have that

$$\text{rk} \ T_f(q)_{L(T)}(\Psi_{T^q}(A)) = m.$$
Figure 3. Construction of the trunk and the boughs of a given tree $T$. Black and white dots represent the leaves in $L_1$ and $L_2$, respectively. Notice that some $T_{i,j}$ may be reduced to the vertex $u_{i,j}$. Indeed, this happens if and only if $u_{i,j} \in L_i$.

**Proof.** First of all, notice that $\text{rk} T f_{(q)}|_{L(T)}(\psi) \leq m$ for all $\psi \in L(T^q)^G$ and that there is a non-empty open set $U \subset L(T^q)^G$ where the above inequality holds. Indeed, if $T f_{(q)}|_{L(T)}(\psi) = (\psi_1, \ldots, \psi_s)$ it is enough to take $U = \cap_{i=1}^s U_i$, where each $U_i$ is defined by asking that $\text{rk} \psi_i = m_i$. Every $U_i$ is a dense open set in $L(T)^G$, and so is $U$.

To reach the claim we only have to prove that $\Psi_{T^q}^{-1}(U)$ is not empty. To this aim, it will be enough to consider the no-mutation presentation $1 = \{1_e\}_{e \in E(T^q)}$. The linear map $\text{flat}_{(q)}|_{L(T)} \Psi_{T^q}(1) : W \to \otimes_{L(T)} W$ defined by $b \mapsto b \otimes \ldots \otimes b$ has rank equal to $\dim(W)$. By virtue of (2.17), we infer that $1 \in \Psi_{T^q}^{-1}(U)$ and we are done. $\square$

Now, we come back to the general case. So, let $T$ be a phylogenetic tree on $(G,W)$ and let $\beta = L_1 \mid L_2$ be a bipartition of $L(T)$. We introduce some terminology and notation that will be helpful. For the sake of clarity, this notation will not reflect its dependence on $\beta$, but confusion should not arise since the bipartition is fixed throughout this section. Keep the notation introduced at the beginning of this section:

1. For $i = 1, 2$ and $j = 1, \ldots, n_i$, denote by $T_{i,j}$ the minimal phylogenetic subtree of $T$ containing $L_{i,j}$. These subtrees are called the **boughs of $T$ relative to $\beta$**. Every $T_{i,j}$ has a distinguished vertex, denoted by $u_{i,j}$, which has degree two. All the remaining interior vertices have degree 3. For $i = 1, 2$, write $L_i^R = \{u_{i,j}\}_{j=1,\ldots,n_i}$.

2. The **trunk of $T$ relative to $\beta$**, denoted by $T_R$, is the phylogenetic tree on $(G,W)$ obtained when removing all the boughs from $T$. Equivalently, $T_R$ is the minimal subtree of $T$ containing all the $u_{i,j}$, so that $L(T_R) = L_1^R \cup L_2^R$.

See figure 3 for an example of this construction.
Notice that $T_R$ is reduced to a 2-leaf tree if and only if $\beta$ is an edge split of $T$. Notice also that every cherry in $T_R$ is composed of one leaf in $L_1^R$ and one leaf in $L_2^R$.

**Proof of Proposition 3.1.** Every $G$-evolutionary presentation $A \in \text{Par}_G(T)$ induces by restriction a $G$-evolutionary presentation $A^R$ in the trunk $T_R$ and $G$-evolutionary presentations $A_{i,j}$ in the boughs $T_{i,j}$. Actually, the mappings $A \mapsto A^R$ and $A \mapsto A_{i,j}$ define continuous maps

$$
\pi_R : \text{Par}_G(T) \to \text{Par}_G(T_R) \quad \pi_{i,j} : \text{Par}_G(T) \to \text{Par}_G(T_{i,j}).
$$

Given $A \in \text{Par}_G(T)$, we proceed to decompose $\Psi_T(A)$ in terms of tensors associated to the trunk and the boughs of $T$. To this aim and for every $i, j$, consider the tree $T_{i,j}^{u_{i,j}}$ with the vertex $u_{i,j}$ observed in it (see section 2.2). It is straightforward to check that $T$ is recovered by joining these boughs to the trunk:

$$
T = T_{1,1}^{u_{1,1}} \ast \ldots \ast (T_{1,n_1}^{u_{1,n_1}} \ast (T_{2,1}^{u_{2,1}} \ast \ldots \ast (T_{2,n_2}^{u_{2,n_2}} \ast T_R) \ldots)) \ldots.
$$

Regarding $A_{i,j}$ as a $G$-evolutionary presentation of $T_{i,j}^{u_{i,j}}$, write $\varphi_{i,j}(A) \in \mathcal{L}(T_{i,j}^{u_{i,j}})$ for the image of $A_{i,j}$ by the map $\Psi_{T_{i,j}}^{u_{i,j}}$ defined in Definition 2.21. Then write

$$
\varphi_A^1 = \otimes_{j=1}^{n_1} \varphi_{1,j}(A) \in (\otimes_{L_R \cup L_1} W)^G \\
\varphi_A^2 = \otimes_{j=1}^{n_2} \varphi_{2,j}(A) \in (\otimes_{L_R \cup L_2} W)^G \\
\varphi_A^R = \Psi_{T_R}(A^R) \in \mathcal{L}(T_R)^G.
$$

From the construction of these three tensors, it is clear that (see Notation 2.5):

$$
\Psi_T(A) = \varphi_A^1 \ast \varphi_A^R \ast \varphi_A^2.
$$

Write $\beta_1 = L_1 \mid L_1^R$, $\beta_2 = L_2 \mid L_2$ and $\beta_R = L_1^R \mid L_2^R$. By applying (2.19) we infer the following equality of maps

$$
Tf_\beta(\Psi_T(A)) = Tf_\beta(\varphi_A^1)Tf_\beta(\varphi_A^R)Tf_\beta(\varphi_A^2)
$$

and from it, the inequality $\text{rk} \ Tf_\beta(\Psi_T(A)) \leq m_{\beta,T}$. Next, we prove that the equality actually holds for a generic $G$-evolutionary presentation $A$ of $T$. It is straightforward to check that this will imply that $\text{rk} \ Tf_\beta(\Psi_T(A)) = m_{\beta,T}$ (use for instance the Frobenius inequality, see Section 2.9.6 of [Eve80]).

First of all, we infer from Lemma 3.3 that there is a dense open set $V_R \subset \text{Par}_G(T_R)$ such that for every $B \in V_R$, $\text{rk} \ Tf_B(\Psi_{T_R}(B)) = m_{\beta_R,T_R}$. Since the map $\pi_R : \text{Par}_G(T) \to \text{Par}_G(T_R)$ is surjective, the set

$$
U_R := \pi_R^{-1}(V)
$$

is a non-empty Zariski open set in $\text{Par}_G(T)$. 

Similarly, for every $i = 1, 2$ and $j = 1, 2, \ldots, n_i$, let $V_{i,j} \subset \text{Par}_G(T_{i,j})$ be the dense open set defined by Lemma 3.4 applied to $T_{i,j}^{u_{i,j}}$ and $U_{i,j} = \pi_{i,j}^{-1}(V_{i,j})$. Since $\text{Par}_G(T)$ is irreducible, it is clear that

$$U_i = \bigcap_{j=1}^{n_i} U_{i,j}, \quad i = 1, 2$$

is non-empty and open. On the other hand, for any $A \in \text{Par}_G(T)$, we have

$$T_{f,\beta i}(\varphi_{i,1}(A) \otimes \cdots \otimes \varphi_{i,n_i}(A)) = \otimes_{j=1}^{n_i} T_{f,L_{i,j}}(\varphi_{i,i}(A))$$

and therefore (see for instance [Eve80])

$$\text{rk } T_{f,\beta i}(\varphi_{i,i}^A) = \prod_{j=1}^{n_i} \text{rk } T_{f,L_{i,j}}(\varphi_{i,i}(A)) = m(n_i).$$

Thus, if $A \in U_i$, the rank of $T_{f,L_{1,2}}(\Psi(A))$ is maximal.

To finish the proof it is enough to take

$$U_\beta = \Psi_T(U_1 \cap U_R \cap U_2) \subset V_T.$$ 

Finally, if $\beta = L_1 \mid L_2$ is an edge split, then $n_1 = n_2 = 1$ and $T_R$ is 2-leaf tree. It follows that $m_{\beta,T} = m$. This proves (i). If $\beta$ is not an edge split, it is clear that $n_1, n_2 \geq 2$ and the claim of (ii) follows by Lemma 2.12. □

**Remark 3.5.** The preceding proof actually shows that the dense open set $U_{L_1 \mid L_2} \subset \text{Par}_G(T)$ cuts the set of stochastic parameters, i.e.

$$U_{L_1 \mid L_2} \cap \prod_{e \in E(T)} \Delta^G \neq \emptyset,$$

where $\Delta^G$ is the set of Markov matrices, that is, matrices whose entries are all non-negative and whose columns sum to 1. Indeed, as suggested by Lemma 3.3 and Lemma 3.4, it is enough to take $A \in \text{Par}_G(T)$ with $A_e = \sum_{b \in B} b \otimes b$ whenever $e \in E(T_R)$ is terminal or $e \in E(T_{i,j})$ for some $i, j$, and $A_e$ a generic Markov matrix, otherwise.

Proposition 3.1 suggests the following definitions.

**Definition 3.6.** If $L_1 \mid L_2$ is a bipartition of $L(T)$, the **ideal of $L_1 \mid L_2$**, denoted by $I_{L_1 \mid L_2}$, is the ideal in the coordinate ring of $\mathcal{L}(T)^G$ defined by the conditions

$$\text{rk } T_{f_{L_1 \mid L_2}}(\psi) \leq m$$

being $\psi \in \mathcal{L}(T)^G$ a tensor of indeterminates. Equivalently, $I_{L_1 \mid L_2}$ is generated by the $(m_t + 1)$-minors of the $t$-th box of $T_{f_{L_1 \mid L_2}}(\psi) \in M_{m(t_1),m(t_2)}$, for $t = 1, \ldots, s$ (see Notation 2.16).
RELEVANT PHYLOGENETIC INVARIANTS...

Notation 3.7. Let \( T \) be a phylogenetic tree on \((G,W)\) and let \( e \) be an edge of \( T \) that splits the leaves into two sets \( L_1 \) and \( L_2 \) of cardinality \( l_1 \) and \( l_2 \), respectively. The ideal \( I_{L_1|L_2} \) will be also denoted as \( I_e \). Due to Proposition 3.1 we have that if \( e \) belongs to \( E(T) \), then \( I_e \subseteq \mathcal{I}(T) \).

Definition 3.8. The edge invariants of \( T \) are the elements of the ideal \( \sum_{e \in E(T)} I_e \).

Proposition 3.1 proves that edge invariants are phylogenetic invariants, that is, elements in \( \mathcal{I}(T) \) that do not vanish on all points of \( \bigcup_T V(T) \) where the union runs over all trivalent tree topologies. Indeed, given a \( G \)-spaced tree \( T_0 \) and an edge \( e \in E(T_0) \), there exist trivalent trees that do not have \( e \) as an edge split and so \( I_e \) is not contained in \( \mathcal{I}(\bigcup_T V(T)) \).

It is worth highlighting that using Proposition 3.1 we also obtain the generic identifiability of the tree topology for equivariant models. The tree topology of a model of sequence mutation is said to be generically identifiable if for generic choices of stochastic parameters \( A \in \prod_{e \in E(T)} \Delta^G, A' \in \prod_{e \in E(T')} \Delta^G \) (see Remark 3.5), \( \Psi_T(A) = \Psi_{T'}(A') \) implies \( T = T' \) (see for instance [AR06]). In order to prove this kind of results, one only has to show the corresponding irreducible varieties \( V(T) \) and \( V(T') \) are not contained one into the other. We obtain the following result that was already known for the general Markov model (see [Ste94]) and for group-based models [SHSE92].

Corollary 3.9. The tree topology is generically identifiable in all equivariant evolutionary models.

**Proof.** Let \( T, T' \) be two different trivalent phylogenetic tree on \((G,W)\). Then there is an edge split \( e \) in \( T \) that is not an edge split in \( T' \). By Proposition 3.1 there exists an element \( f \) in \( I_e \) (and therefore in \( \mathcal{I}(T) \)) that does not belong to \( \mathcal{I}(T') \). In terms of varieties this proves that \( V(T') \subsetneq V(T) \), and that \( V(T) \subsetneq V(T') \) is proven similarly. As \( V(T) \) and \( V(T') \) are irreducible varieties, this shows that they meet properly. \( \square \)

4. Phylogenetic Invariants

The purpose of this section is to prove that, for phylogenetic reconstruction, the only relevant invariants are the edge invariants introduced in the previous section. This is a natural result if one takes into account the Splits Equivalence Theorem in combinatorics (see Theorem 4.1 below). Let \( T \) be the set of trivalent tree topologies with leaf set \( \{v_1, v_2, \ldots, v_n\} \). Two bipartitions \( L_1|L_2, M_1|M_2 \) of a set \( L \) are said to be compatible if at least one of the four intersections \( L_1 \cap M_1, L_1 \cap M_2, L_2 \cap M_1, L_2 \cap M_2 \) is empty. For example, if \( L_1|L_2, M_1|M_2 \) are two edge splits of the same tree \( T \), then they are compatible. We recall that any trivalent tree on \( n \) leaves has \( 2n - 3 \) interior edges.
**Theorem 4.1** ([Bun71], [PS05, Theorem 2.35]). A collection $\mathcal{B}$ of $2n - 3$ bipartitions is pairwise compatible if and only if there exists a tree $T \in \mathcal{T}$ such that $\mathcal{B}$ is the set of edge splits of $T$. Moreover, if such a tree $T$ exists then it is unique.

In order to make our result concerning phylogenetic invariants more precise we need to introduce some notation.

We fix $G \subset \mathfrak{S}_k$ and $W$ as in section 2 and each topology $T \in \mathcal{T}$ will be considered as a phylogenetic tree on $(G, W)$. Then all trees $T$ in $\mathcal{T}$ have the same space of $G$-tensors which will be denoted by $\mathcal{L} = (\bigotimes_{i=1}^n W)^G$.

**Definition 4.2.** Let $\mathbf{o}$ be an $s$-tuple and let $\beta = L_1 \mid L_2$ be a bipartition of $\{v_1, v_2, \ldots, v_n\}$. Then we let $D^\beta_{\leq \mathbf{o}}$ be the subvariety of $\mathcal{L}$ defined as

$$D^\beta_{\leq \mathbf{o}} = \{ \psi \in \mathcal{L} \mid \text{rk } T f_\beta(\psi) \leq \mathbf{o} \}$$

and, if the thin flattening of $\psi \in \mathcal{L}$ is $T f_\beta(\psi) = (\psi_1, \psi_2, \ldots, \psi_s)$, we define $D^\beta_{< \mathbf{o}}$ to be the set

$$D^\beta_{< \mathbf{o}} = \{ \psi \in \mathcal{L} \mid \text{rk } \psi_j < o_j \text{ for some } j \}.$$  

For example, $D^\beta_{\leq \mathbf{m}}$ coincides with the set of zeroes $Z(I_{L_1, L_2})$. Notice that both $D^\beta_{\leq \mathbf{o}}$ and $D^\beta_{< \mathbf{o}}$ are algebraic sets although the second is not irreducible.

**Notation 4.3.** Given a tree $T \in \mathcal{T}$ and using the notation of Proposition 3.1 for each bipartition $\beta = L_1 \mid L_2$ of $\{v_1, v_2, \ldots, v_n\}$, we call $m_{\beta, T}$ the maximum rank that $T f_\beta(\psi)$ can have if $\psi$ belongs to $V(T)$. Then Proposition 3.1 shows that

$$V(T) \subseteq D^\beta_{\leq m_{\beta, T}}$$

and that $V(T) \setminus D^\beta_{< m_{\beta, T}}$ is a dense open subset of $V(T)$ for any bipartition $\beta = L_1 \mid L_2$. We call this open subset $U_{T, \beta}$, so that $U_{T, \beta} = V(T) \setminus D^\beta_{< m_{\beta, T}}$ is the locus of tensors $\psi \in V(T)$ that satisfy $\text{rk } T f_\beta(\psi) = m_{\beta, T}$. We define $U_T = \cap_{\beta} U_{T, \beta}$, where the intersection is taken among all bipartitions of $\{v_1, v_2, \ldots, v_n\}$. As $V(T)$ is an irreducible variety, $U_T$ is still a dense open subset of $V(T)$ and it corresponds to the set of points in $V(T)$ whose flattening $T f_\beta(\psi)$ along any partition $\beta$ of the set of leaves of $T$ has the expected rank $m_{\beta, T}$.

With this set up in mind, the main result of this paper is the following,

**Theorem 4.4.** For each $T \in \mathcal{T}$, let $U_T \subseteq V(T)$ be the dense open set defined above. Let $p$ be a point in $\bigcup_{T \in \mathcal{T}} U_T \subseteq \mathcal{L}$ and let $T_0$ be any tree in $\mathcal{T}$. Then, $p$ belongs to $V(T_0)$ if and only if $p$ belongs to the set of zeroes $Z(\sum_{e \in E(T_0)} I_e)$.

**Remark 4.5.** As we pointed out in the introduction, this result says that for a general point on $\bigcup_{T \in \mathcal{T}} V(T)$, it is enough to evaluate the edge invariants to decide to which variety $V(T)$ the point actually belongs to.

This result would still hold for non-trivalent trees when imposing that all trees in the corresponding set $\mathcal{T}$ have the same collection of degrees at interior vertices.
After all the technical issues in section 3, the proof of Theorem 4.4 is now straightforward.

**Proof of 4.4.** By Proposition 3.1 we already know that $\sum_{e \in E(T_0)} I_e \subseteq \mathcal{I}(T_0)$, therefore if $p \in V(T_0)$, we immediately have that $p$ belongs to $Z(\sum_{e \in E(T_0)} I_e)$.

Conversely, let $p \in \bigcup_{T \in \mathcal{T}} U_T$. Then $p$ belongs to $U_T \subset V(T)$ for a certain $T \in \mathcal{T}$, so that $rk T f_\beta(p) = m_{\beta,T}$ for any bipartition $\beta$ of $\{v_1, v_2, \ldots, v_n\}$. On the other hand, if $p \in Z(\sum_{e \in E(T_0)} I_e)$, then $p \in Z(I_e)$ for any $e \in E(T_0)$ and hence, $rk T f_\beta(p) \leq m$ for all $e \in E(T_0)$. This implies that $m_{e,T} \leq m$ for all $e \in E(T_0)$, which can only happen if $e$ is a split of $T$ for all $e \in E(T_0)$ (see Proposition 3.1). But two trivalent trees $T$ and $T_0$ on $n$ leaves have the same collection of splits if and only if $T = T_0$ (see Theorem 4.1), so the proof is concluded. \(\Box\)

**Remark 4.6.** Theorem 4.4 also says that the intersection $U_T \cap U_{T'}$ is empty for any $T \neq T' \in \mathcal{T}$. However, there exists points in $V(T) \cap V(T')$ for any $T \neq T'$. Indeed, it is enough to consider $\psi_T(A)$ where $A$ is the no-mutation presentation; then $\psi_T(A)$ lies in $V(T')$ for all $T'$. This proves that $\bigcap_{T} V(T)$ is not empty but one can also prove that, if $n \geq 5$, for any two different tree topologies $T_1, T_2$ one has $V(T_1) \cap V(T_2) \neq \bigcap_{T} V(T)$.

In the next Corollary we give an open subset $U$ defined intrinsically from the ambient space $\mathcal{L}$ such that $U \cap \bigcup_{T \in \mathcal{T}} V(T) = \bigcup_{T \in \mathcal{T}} U_T$. This is relevant for biological applications because then we will be able to check whether the given data point lies (or rather is close to) in $\bigcup_{T} U_T$. From now on let $\mathcal{B}$ be the set of all bipartitions of $\{v_1, \ldots, v_n\}$.

**Corollary 4.7.** Let $U = \bigcup_{T \in \mathcal{T}} \bigcap_{\beta \in \mathcal{B}} (\mathcal{L} \setminus D_{<m_{\beta,T}}^\beta)$. Then

$$U \cap \bigcup_{T \in \mathcal{T}} V(T) = \bigcup_{T \in \mathcal{T}} U_T$$

and if $p$ is a point in $U \cap \bigcup_{T \in \mathcal{T}} V(T)$ and $T_0$ is any tree in $\mathcal{T}$, then $p$ belongs to $V(T_0)$ if and only if $p$ belongs to the set of zeroes $Z(\sum_{e \in E(T_0)} I_e)$.

**Proof.** We just need to prove that $U \cap (\bigcup_{T \in \mathcal{T}} V(T)) = \bigcup_{T \in \mathcal{T}} U_T$ because the other assertion follows from Theorem 4.4.

We have $U \cap (\bigcup_{T \in \mathcal{T}} V(T)) = \bigcup_{T,T'} V(T) \cap (\bigcap_{\beta} \mathcal{L} \setminus D_{<m_{\beta,T'}}^\beta)$. If $T \neq T'$ this intersection is the empty as we can see taking $\beta$ an edge split of $T$ but not of $T'$. Hence we obtain $U \cap (\bigcup_{T \in \mathcal{T}} V(T)) = \bigcup_{T} V(T) \cap (\bigcap_{\beta} \mathcal{L} \setminus D_{<m_{\beta,T}}^\beta)$, which is precisely $\bigcup_{T} U_T$. \(\Box\)

In terms of ideals, Theorem 4.4 says the following:
Corollary 4.8. Let \( R \) be the polynomial ring of \( \mathcal{L} \) and let \( f \) be any element in

\[
\left( \sum_{T \in \mathcal{B}} \bigcap_{\beta \in \mathcal{B}} \mathcal{I}(D_{< m_{\beta,T}}) \right) \setminus \bigcap_{T} \mathcal{I}(T).
\]

Then, the following equality holds in the localized ring \((R \setminus \bigcap_{T} \mathcal{I}(T))_{\overline{T}}\)

\[
\left( \left( \mathcal{I}(T_0) \cap \bigcap_{T} \mathcal{I}(T) \right)_{\overline{T}} = \left( \text{rad} \left( \sum_{e \in E(T_0)} I_e \right) \cap \bigcap_{T} \mathcal{I}(T) \right)_{\overline{T}}.\right.
\]

PROOF. If we are given an \( f \) as above, then \( U_f := \mathcal{L} \setminus \{ f = 0 \} \) is contained inside the open set \( U \) defined in Corollary 4.7. Indeed, an \( f \) as above is contained inside \( \text{rad}(\sum_{T \in \mathcal{B}} \bigcap_{\beta} \mathcal{I}(D_{< m_{\beta,T}})) \) which is equal to \( \mathcal{I}(\bigcap_{T} \cup_{\beta} D_{< m_{\beta,T}}) \). Therefore \( \bigcap_{T} \cup_{\beta} D_{< m_{\beta,T}} \subset \{ f = 0 \} \) and \( U_f \subset \mathcal{L} \setminus \bigcap_{T} \cup_{\beta} D_{< m_{\beta,T}} = U \).

In particular, \( U_f \cap (\cup_{T} V(T)) \) is contained inside \( \cup_{T} U_T \). Therefore in \( U_f \) we still have that the variety \( V(T_0) \) is defined inside \( \cup_{T \in \mathcal{T}} V(T) \) by \( \sum_{e \in E(T_0)} I_e \). Hence in terms of ideals in \( R_f \) we obtain the equality above. \( \square \)

We do not know whether \( \sum_{e \in E(T_0)} I_e \) is a radical ideal so we cannot remove \( \text{rad} \) from the expression above. We pose the following question:

**Question 4.9.** Given a set \( S \) of compatible splits, is \( \sum_{\beta \in S} I_{\beta} \) radical?

**Remark 4.10.** In order to check whether Theorem 4.4 can be applied to a given data point \( p \in \mathcal{L} \), it is enough to check that \( f(p) \neq 0 \) for a generic \( f \) in

\[
\left( \sum_{T \in \mathcal{B}} \bigcap_{\beta} \mathcal{I}(D_{< m_{\beta,T}}) \right) \setminus \bigcap_{T} \mathcal{I}(T).
\]

Such a polynomial \( f \) should be chosen a priori, so that when dealing with data one does not need to compute this ideal.

**Remark 4.11.** It is interesting to explore whether \( U_T \) can be defined by a complete intersection in the sense of [CFS08]. This would reduce the number of generators of \( I_e \) to be used in phylogenetic reconstruction. However, this is another issue on which we plan to work in the future.

Although the degrees of a set of generators of the ideal of a phylogenetic tree evolving under the general Markov model or under the strand symmetric model are not known, Theorem 4.4 allows us to give the degrees of those invariants that are relevant in phylogenetic reconstruction. It is worth highlighting that these degrees do not depend on the number of leaves but only on the model and can be computed a priori (see the next sections for the precise examples of evolutionary models).
Corollary 4.12. Let \((G, W)\) be an equivariant evolutionary model and let \(m = (m_1, \ldots, m_s)\) be defined as in section 3. Then, for any tree topology on any number of leaves, the polynomials that are relevant for recovering the tree topology in phylogenetics have degrees in \(\{m_1+1, \ldots, m_s+1\}\). In particular, the relevant phylogenetic invariants for the following evolutionary models have degrees:

- 5 for the general Markov model.
- 3 for the strand symmetric model.
- 2 for the Kimura 3-parameter model.
- 1 or 2 for the Kimura 2-parameter model.
- 1 or 2 for the Jukes-Cantor model.

5. Examples

In this section, we study some well-known evolutionary models in phylogenetics. Let \(B = \{A, C, G, T\}\) be the set of the four nucleotides and take \(W = \langle A, C, G, T \rangle \cong \mathbb{C}^4\) with the bilinear form \((\cdot | \cdot)_W\) that makes \(B\) orthonormal. We consider the group of permutations of 4 elements,

\[
\mathfrak{S}_4 = \text{Sym}\{B\}.
\]

It is generated by \(g_1 = (\text{id}), g_2 = (AC), g_3 = (ACG), g_4 = (ACGT)\) and \(g_5 = (AC)(GT)\), which correspond to the five conjugacy classes of \(\mathfrak{S}_4\). We work with the natural permutation linear representation \(\rho : \mathfrak{S}_4 \to \text{GL}(W)\) given by permuting the coordinates of \(W\):

\[
\begin{align*}
g_1 &\mapsto \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, & g_2 &\mapsto \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, & g_3 &\mapsto \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \\
g_4 &\mapsto \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, & g_5 &\mapsto \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\end{align*}
\]

Write \(\chi = \text{Tr}(\rho(\cdot))\) for the character associated to it. We shall consider different subgroups of \(\mathfrak{S}_4\), each one of them giving rise to a different equivariant model, according to the following diagram (we use the following shortenings: GMM for the general Markov model, K81 for the Kimura 3 parameter model, K80 for the Kimura
2 parameter model, CS05 for the strand symmetric model and JC69 for the Jukes-Cantor model):

\[
\begin{array}{c}
\{\text{id}\} \\
((AC)(GT), (AG)(CT)) \\
((ACGT), (AG)) \\
\mathbb{S}_4 \\
\end{array}
\begin{array}{c}
\text{GMM} \\
K81 \\
JC69 \\
\end{array}
\begin{array}{c}
\{v_1, v_2, v_3, v_4\} \\
\{v_3, v_4\} \\
\{v_1, v_2\} \\
\end{array}
\]

Our aim here is to describe in a unified fashion the edge invariants associated to these models for the case of a quartet tree topology \( T \), with leaves \( v_1, v_2, v_3, v_4 \). Write \( e = L_1 \mid L_2 \) for the edge split corresponding to \( e \), so that \( L_1 = \{v_1, v_2\} \) and \( L_2 = \{v_3, v_4\} \).

**Remark 5.1.** When the subgroup \( G \subset \mathbb{S}_4 \) is abelian, the usual product of complex numbers induces on \( \Omega_G \) a group structure. Then, if \( \{u_1^i, \ldots, u_m^i\} \) is a basis for \( W[\omega] \), for every \( \omega \in \Omega_G \), we have that

\[
\{u_{j_1}^{i_1} \otimes \cdots \otimes u_{j_l}^{i_l} \mid \omega_{i_1} \cdots \omega_{i_l} = \omega \}
\]

is a \( \mathbb{C} \)-basis for \( (\otimes^l W)[\omega] \).

### 5.1. General Markov model

As a first example, consider the trivial subgroup \( \{1\} \subset \mathbb{S}_4 \). The corresponding equivariant model is the general Markov model, which is the most general model in the Felsenstein hierarchy (see Ch.4 in [PS05](#)). Invariants for this model have been studied by Allman and Rhodes in [AR03](#) and [AR07](#). In this case, there is only one irreducible representation \( \omega : G \to \mathbb{C} \) defined by mapping \( (1) \) to 1. The character table is

| \( \Omega(1) \) | \( \text{id} \) | 1 | 4 |
|----------------|---------------|---|---|
| \( \omega \)   | 1             |   |   |
| \( \chi \)     | 4             |   |   |

It follows that \( \chi = 4 \omega \). Keeping the notation introduced in [2.1](#) we have \( m = (4) \) and \( W = W[\omega] \cong N_\omega \otimes \mathbb{C}^4 \).
Now, for the case of four leaves, we have $\chi^2 = 16\omega$ and $m(2) = (16)$. Then, the ideal $I_e$ is defined by the condition

$$\text{rk}(M) \leq (4)$$

where $M \in \text{Hom}_G((W \otimes W)[\omega], (W \otimes W)[\omega]) \cong \text{Hom}_C(C^{16}, C^{16})$ is a matrix of indeterminates whose columns and rows are indexed by the set $\{X_1 \otimes X_2 \}_{X_1, X_2 \in B}$. The ideal $I_e$ obtained by imposing the above rank condition is generated by $\binom{16}{5} \binom{16}{5}$ polynomials of degree 5.

5.2. Strand symmetric model. Take $G = \langle (AT)(CG) \rangle$, which is isomorphic to $\mathbb{Z}/2\mathbb{Z}$. The equivariant matrices for this group have the following structure:

$$
\begin{pmatrix}
 a & b & c & d \\
 e & f & g & h \\
 h & g & f & e \\
 d & c & b & a
\end{pmatrix}
$$

The equivariant model associated to $G$ is the strand symmetric model introduced in [CS05]. There are two irreducible characters $\omega_1, \omega_2$, and the character table is

| $\Omega_G$ | id | $(AT)(CG)$ |
|------------|----|------------|
| $\omega_1$ | 1  | 1          |
| $\omega_2$ | 1  | -1         |
| $\chi$     | 4  | 0          |

Notice that since $G$ is abelian, all the irreducible representations have dimension one. It follows that $\chi = 2\omega_1 + 2\omega_2$. Thus, $m = (2, 2)$ and we have a decomposition ([FH91 Corollary 2.14])

$$W = W[\omega_1] \oplus W[\omega_2],$$

where $W[\omega_1] \cong N_{\omega_1} \otimes C^2$ and $W[\omega_2] \cong N_{\omega_2} \otimes C^2$. Indeed, if we write

$$u_1 = A + T \quad u_2 = C + G \quad v_1 = A - T \quad v_2 = C - G,$$

we have

$$W[\omega_1] = \langle u_1, u_2 \rangle_C \quad W[\omega_2] = \langle v_1, v_2 \rangle_C.$$

Now, we focus on the case of the tree with four leaves. We have $\chi^2 = 8\omega_1 + 8\omega_2$, so $m(2) = (8, 8)$. Moreover, using that $G$ is abelian (see Remark 5.1)

$$W \otimes W[\omega_1] = \langle u_1 \otimes u_1, u_1 \otimes u_2, u_2 \otimes u_1, u_2 \otimes u_2, v_1 \otimes v_1, v_1 \otimes v_2, v_2 \otimes v_1, v_2 \otimes v_2 \rangle$$
$$W \otimes W[\omega_2] = \langle u_1 \otimes v_1, u_1 \otimes v_2, u_2 \otimes v_1, u_2 \otimes v_2, v_1 \otimes u_1, v_1 \otimes u_2, v_2 \otimes u_1, v_2 \otimes u_2 \rangle$$

Then, the ideal $I_e$ is defined by the conditions

$$\text{rk} \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix} \leq (2, 2)$$
where

\[
M_1 = \begin{pmatrix}
q_{u_1u_1u_1} & q_{u_1u_2u_1} & q_{u_1u_2u_2} & q_{u_1u_1v_1} & q_{u_1u_1v_2} & q_{u_1u_2v_1} & q_{u_1u_2v_2} \\
q_{u_2u_1u_1} & q_{u_2u_1u_2} & q_{u_2u_2u_1} & q_{u_2u_2u_2} & q_{u_2u_1v_1} & q_{u_2u_1v_2} & q_{u_2u_2v_1} \\
q_{u_2u_2u_1} & q_{u_2u_2u_2} & q_{u_2u_2u_1} & q_{u_2u_2v_1} & q_{u_2u_2v_2} & q_{u_2u_1v_2} & q_{u_2u_1v_1} \\
q_{v_1v_1u_1} & q_{v_1v_1u_2} & q_{v_1v_1v_2} & q_{v_1v_1v_1} & q_{v_1v_2v_2} & q_{v_2v_1v_2} & q_{v_2v_1v_1} \\
q_{v_1v_2u_1} & q_{v_1v_2u_2} & q_{v_1v_2v_2} & q_{v_1v_2v_1} & q_{v_2v_1v_2} & q_{v_2v_1v_1} & q_{v_2v_2v_2} \\
q_{v_2v_1u_1} & q_{v_2v_1u_2} & q_{v_2v_1v_2} & q_{v_2v_1v_1} & q_{v_2v_2v_2} & q_{v_2v_2v_1} & q_{v_2v_2v_2} \\
q_{v_2v_2u_1} & q_{v_2v_2u_2} & q_{v_2v_2v_2} & q_{v_2v_2v_1} & q_{v_2v_2v_2} & q_{v_2v_2v_2} & q_{v_2v_2v_2}
\end{pmatrix}
\]

\[
M_2 = \begin{pmatrix}
q_{v_1v_1v_1} & q_{v_1v_1v_2} & q_{v_1v_2v_2} & q_{v_1v_1v_1} & q_{v_1v_1v_2} & q_{v_1v_2v_2} \\
q_{v_2v_1v_1} & q_{v_2v_1v_2} & q_{v_2v_2v_2} & q_{v_2v_1v_1} & q_{v_2v_1v_2} & q_{v_2v_2v_2} \\
q_{v_2v_2v_1} & q_{v_2v_2v_2} & q_{v_2v_2v_1} & q_{v_2v_2v_2} & q_{v_2v_2v_2} & q_{v_2v_2v_2} \\
q_{v_1v_1v_1} & q_{v_1v_1v_2} & q_{v_1v_2v_2} & q_{v_1v_1v_1} & q_{v_1v_1v_2} & q_{v_1v_2v_2} \\
q_{v_1v_2v_1} & q_{v_1v_2v_2} & q_{v_1v_2v_2} & q_{v_1v_2v_2} & q_{v_1v_2v_2} & q_{v_1v_2v_2} \\
q_{v_2v_1v_1} & q_{v_2v_1v_2} & q_{v_2v_1v_2} & q_{v_2v_1v_2} & q_{v_2v_1v_2} & q_{v_2v_1v_2} \\
q_{v_2v_2v_1} & q_{v_2v_2v_2} & q_{v_2v_2v_2} & q_{v_2v_2v_2} & q_{v_2v_2v_2} & q_{v_2v_2v_2}
\end{pmatrix}
\]

and \(q_{x,y,z,t}\) are the coordinates in the basis \(x \otimes y \otimes z \otimes t\). We see that \(I_c\) is generated by \(\binom{8}{3}(\binom{8}{3}) + \binom{8}{3}(\binom{8}{3}) = 6272\) polynomials of degree 3.

5.3. Kimura 3-parameter model. Take \(G = \langle (AC)(GT), (AG)(CT) \rangle\), which is also isomorphic to \(\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}\). The equivariant matrices for this group have the following structure:

\[
\begin{pmatrix}
a & b & c & d \\
b & a & d & c \\
c & d & a & b \\
d & c & b & a
\end{pmatrix}
\]

In this case, the equivariant model is the Kimura 3-parameter model introduced in [Kim81]. We write \(\omega_A, \omega_C, \omega_G, \omega_T\) for the irreducible characters of \(G\). The corresponding table is

| \(\Omega_G\) | id | (AC)(GT) | (AG)(CT) | (AT)(CG) |
|-------------|----|----------|----------|----------|
| \(\omega_A\) | 1  | 1        | 1        | 1        |
| \(\omega_C\) | 1  | -1       | 1        | -1       |
| \(\omega_G\) | 1  | 1        | -1       | -1       |
| \(\omega_T\) | 1  | -1       | -1       | 1        |
| \(\chi\)    | 4  | 0        | 0        | 0        |

It follows that \(\chi = \omega_A + \omega_C + \omega_G + \omega_T\) and so, \(m = (1,1,1,1)\)

\[W = W[\omega_A] \oplus W[\omega_C] \oplus W[\omega_G] \oplus W[\omega_T],\]
where

\[ W[\omega_k] \cong N_{\omega_k} \quad W[\omega_c] \cong N_{\omega_c} \quad W[\omega_g] \cong N_{\omega_g} \quad W[\omega_T] \cong N_{\omega_T}. \]

In fact, if we write

\[
(5.1) \quad \bar{A} = A + C + G + T \quad \bar{C} = A + C - G - T \\
\bar{G} = A - C + G - T \quad \bar{T} = A - C - G + T
\]

we have

\[
W[\omega_k] = \langle \bar{A} \rangle \quad W[\omega_c] = \langle \bar{C} \rangle \quad W[\omega_g] = \langle \bar{G} \rangle \quad W[\omega_T] = \langle \bar{T} \rangle
\]

We remark that the basis \( \{\bar{A}, \bar{C}, \bar{G}, \bar{T}\} \) is the image of \( \{A, C, G, T\} \) by the Fourier transform described in [CFS08] or [CGS05].

Since \( \chi^2 = 4\omega_k + 4\omega_c + 4\omega_g + 4\omega_T \), we have \( m(2) = (4, 4, 4, 4). \) In virtue of Remark 5.1,

\[
W \otimes W[\omega_k] = \langle \bar{A} \otimes \bar{A}, \bar{C} \otimes \bar{C}, \bar{G} \otimes \bar{G}, \bar{T} \otimes \bar{T} \rangle \\
W \otimes W[\omega_c] = \langle \bar{A} \otimes \bar{C}, \bar{C} \otimes \bar{A}, \bar{G} \otimes \bar{T}, \bar{T} \otimes \bar{C} \rangle \\
W \otimes W[\omega_g] = \langle \bar{A} \otimes \bar{G}, \bar{C} \otimes \bar{T}, \bar{G} \otimes \bar{A}, \bar{T} \otimes \bar{G} \rangle \\
W \otimes W[\omega_T] = \langle \bar{A} \otimes \bar{T}, \bar{C} \otimes \bar{G}, \bar{G} \otimes \bar{C}, \bar{T} \otimes \bar{A} \rangle
\]

Then, \( I_e \) is given by the conditions

\[
(5.2) \quad \text{rk} \begin{pmatrix} M_\lambda & 0 & 0 & 0 \\ 0 & M_\gamma & 0 & 0 \\ 0 & 0 & M_G & 0 \\ 0 & 0 & 0 & M_T \end{pmatrix} \leq (1, 1, 1, 1)
\]

where \( M_Z \in M_{4,4} \) for all \( Z \in B \), that is,

\[
M_\lambda = \begin{pmatrix} q_{\lambda AA\lambda} & q_{\lambda ACC} & q_{\lambda AGC} & q_{\lambda ATT} \\ q_{\lambda CAA} & q_{\lambda CCC} & q_{\lambda GCG} & q_{\lambda CCT} \\ q_{\lambda GAA} & q_{\lambda GCC} & q_{\lambda GCG} & q_{\lambda GCT} \\ q_{\lambda TAA} & q_{\lambda TCC} & q_{\lambda TCG} & q_{\lambda TTC} \end{pmatrix} \quad M_\gamma = \begin{pmatrix} q_{\gamma AC\gamma} & q_{\gamma ACA} & q_{\gamma ACT} & q_{\gamma ATC} \\ q_{\gamma CAC} & q_{\gamma CCA} & q_{\gamma CAT} & q_{\gamma CTA} \\ q_{\gamma GAC} & q_{\gamma GCA} & q_{\gamma GAT} & q_{\gamma GTC} \\ q_{\gamma TAC} & q_{\gamma TCA} & q_{\gamma TCT} & q_{\gamma TGT} \end{pmatrix} \\
M_G = \begin{pmatrix} q_{\lambda AG\lambda} & q_{\lambda ACG} & q_{\lambda ACG} & q_{\lambda ATG} \\ q_{\lambda GAG} & q_{\lambda GCG} & q_{\lambda GCT} & q_{\lambda GGT} \\ q_{\lambda CGA} & q_{\lambda CGA} & q_{\lambda CGT} & q_{\lambda GGT} \\ q_{\lambda TAG} & q_{\lambda TAG} & q_{\lambda TAG} & q_{\lambda TGT} \end{pmatrix} \quad M_T = \begin{pmatrix} q_{\lambda AT\lambda} & q_{\lambda ATG} & q_{\lambda ATG} & q_{\lambda ATG} \\ q_{\lambda CAT} & q_{\lambda CAT} & q_{\lambda CAT} & q_{\lambda CAT} \\ q_{\lambda GAT} & q_{\lambda GAT} & q_{\lambda GAT} & q_{\lambda GAT} \\ q_{\lambda TAT} & q_{\lambda TAT} & q_{\lambda TAT} & q_{\lambda TAT} \end{pmatrix}
\]

where \( q_{x_1x_2x_3x_4} \) are the coordinates in the basis \( \\{ \bar{x}_1 \otimes \bar{x}_2 \otimes \bar{x}_3 \otimes \bar{x}_4 \}_{x_i \in B} \). The ideal \( I_e \) obtained by imposing the rank conditions of (5.3) is generated by \( \binom{1}{2} \left( \binom{1}{2} \binom{1}{2} + \binom{1}{2} \binom{1}{2} \right) = 144 \) quadrics. However, at any point of \( V(I_e) \) the variety is locally defined by 36 quadrics (see [CFS08] Example 4.9)).
5.4. Kimura 2-parameter model. Take $G = \langle (ACGT), (AG) \rangle$, which is isomorphic to the dihedral group. The equivariant matrices for this group have the following structure:

$$
\begin{pmatrix}
  a & b & c & b \\
  b & a & b & c \\
  c & b & a & b \\
  b & c & b & a \\
\end{pmatrix}
$$

The equivariant model is the Kimura 2-parameter model introduced in [Kim80]. There are 5 irreducible characters $\omega_1, \omega_2, \omega_3, \omega_4, \omega$ and the corresponding table is

| $\Omega_G$ | id | (ACGT) | (AG) | (AG)(CT) | (ATGC) |
|------------|----|--------|------|----------|-------|
| $\omega_1$ | 1  | 1      | 1    | 1        | 1     |
| $\omega_2$ | 1  | 1      | -1   | 1        | 1     |
| $\omega_3$ | 1  | -1     | 1    | 1        | -1    |
| $\omega_4$ | 1  | -1     | -1   | 1        | -1    |
| $\omega$   | 2  | 0      | 0    | -2       | 0     |

Notice that $G$ is not abelian and that the irreducible representation $\omega$ is 2-dimensional. It follows that $\chi = \omega_1 + \omega_3 + \omega$ and so, $m = (1, 0, 1, 0, 1)$ and

$$\
W = W[\omega_1] \oplus W[\omega_3] \oplus W[\omega],
$$

where

$$
W[\omega_1] \cong N_{\omega_1}, \quad W[\omega_3] \cong N_{\omega_3}, \quad W[\omega] \cong N_{\omega}.
$$

In fact, with the notation of (5.1) we have

$$\
W[\omega_1] = \langle A \rangle, \quad W[\omega_3] = \langle G \rangle, \quad W[\omega] = \langle C, T \rangle.
$$

Now, we consider the case of four leaves. We have $\chi^2 = 3\omega_1 + \omega_2 + 3\omega_3 + \omega_4 + 4\omega$, so $m(2) = (3, 1, 3, 1, 4)$. If $\psi \in \mathcal{L}(T)^G$, then

$$
Tf_e(\psi) = \begin{pmatrix}
  s_1 & 0 & 0 & 0 & 0 \\
  0 & s_2 & 0 & 0 & 0 \\
  0 & 0 & s_3 & 0 & 0 \\
  0 & 0 & 0 & s_4 & 0 \\
  0 & 0 & 0 & 0 & s \\
\end{pmatrix} \in M_{m(2), m(2)}
$$

where

$$
S_1 \in M_{5,3} \quad S_2 \in M_{1,1} \quad S_3 \in M_{3,3} \quad S_3 \in M_{1,1} \quad S \in M_{4,4}.
$$

Then, the ideal $I_e$ is given by the condition

$$
(5.3) \quad \text{rk } Tf_{L_1 | L_2}(\psi) \leq (1, 0, 1, 0, 1).
$$

By imposing these rank conditions to the matrix $Tf_{L_1 | L_2}(\psi)$ we obtain $\binom{3}{2}(3) + \binom{1}{1}(1) + \binom{2}{3}(2) + \binom{1}{1}(1) + \binom{4}{3}(2) = 9 + 1 + 9 + 1 + 36 = 56$ invariants: 54 of them are quadrics and 2 of them are linear invariants.
5.5. **Jukes-Cantor model.** Finally, we take the whole group of permutations $\mathcal{S}_4$. The equivariant matrices for this group have the following structure:

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

The equivariant model associated to it is the *Jukes-Cantor model* introduced in [JC69]. The group $\mathcal{S}_4$ has five irreducible characters $\{\omega_i\}_{i=0,...,4}$ (see §2.3 of [FH91]) and the following character table:

| $\Omega_{\mathcal{S}_4}$ | id | (AC) | (ACG) | (ACGT) | (AC)(GT) |
|---------------------------|----|------|------|--------|----------|
| $\omega_0$                | 1  | 1    | 1    | 1      | 1        |
| $\omega_1$                | 1  | -1   | 1    | -1     | 1        |
| $\omega_2$                | 2  | 0    | -1   | 0      | 2        |
| $\omega_3$                | 3  | 1    | 0    | -1     | -1       |
| $\omega_4$                | 3  | -1   | 0    | 1      | -1       |
| $\chi$                    | 4  | 2    | 1    | 0      | 0        |

It follows that

$$
\chi = \omega_0 + \omega_3,
$$

that is, $\chi$ is the sum of the trivial and the *standard* representations. We have $m = (1, 0, 0, 1, 0)$. Thus, there is a decomposition

$$
W = W[\omega_0] \oplus W[\omega_3],
$$

where

$$
W[\omega_0] \cong N_{\omega_0} \otimes C^{m_0} \cong N_{\omega_0} \quad \text{dim } W[\omega_0] = 1
$$

$$
W[\omega_3] \cong N_{\omega_3} \otimes C^{m_3} \cong N_{\omega_3} \quad \text{dim } W[\omega_3] = 3.
$$

In fact, with the notation of (5.1), we have

$$
W[\omega_0] = (\mathbb{A}) \quad W[\omega_3] = (\mathbb{C}, \mathbb{G}, \mathbb{T}).
$$

The ideal $I_e$ is generated by the $(m_j + 1)$-minors of the $j$-th box of $T_f e(\psi)$ with $j = 1, 2, \ldots, 5$. On the other hand, it is straightforward to see that $\chi^2 = 2\omega_0 + \omega_2 + 3\omega_3 + \omega_4$, so $m(2) = (2, 0, 1, 3, 1)$ and we have

$$
(W \otimes W)[\omega_0] = \langle q_{AA}, q_{CC} + q_{GG} + q_{TT} \rangle
$$

$$
(W \otimes W)[\omega_2] = \langle q_{CC} - q_{GG}, q_{CC} - q_{TT} \rangle
$$

$$
(W \otimes W)[\omega_3] = \langle q_{AC}, q_{AG}, q_{GT}, q_{GG}, q_{TA}, q_{CT} + q_{TC}, q_{CG} + q_{GC}, q_{GT} + q_{TG} \rangle
$$

$$
(W \otimes W)[\omega_4] = \langle q_{CT} - q_{TC}, q_{CG} - q_{GC}, q_{GT} - q_{TG} \rangle
$$
and $q_{XY} = q_X \otimes q_Y$, for any $X, Y \in B$. Now, if $\psi \in L(T)^{\mathfrak{S}_4}$ we have

$$Tf_e(\psi) = \begin{pmatrix}
S_0 & 0 & 0 & 0 \\
0 & S_2 & 0 & 0 \\
0 & 0 & S_3 & 0 \\
0 & 0 & 0 & S_4 \\
\end{pmatrix} \in M_{m(2), m(2)}$$

where

$$S_0 \in M_{2,2} \quad S_2 \in M_{1,1} \quad S_3 \in M_{3,3} \quad S_4 \in M_{1,1}.$$  

For instance, we have

$$S_0 = \begin{pmatrix}
q_{AAAA} & q_{AACC} + q_{AGGG} + q_{ATT} \\
q_{CCAA} + q_{GGAA} + q_{TTAA} & q_{CCCC} + q_{CGGC} + q_{GGTC} + q_{TTAC} + q_{CTTT} + q_{TTTT}
\end{pmatrix}$$

while

$$S_2 = (q_{CCCC} - q_{CCGG} - q_{GGCC} + q_{GGGG}).$$

Now, given $\psi \in L(T)^{\mathfrak{S}_4}$, we have $\psi \in V(T)$ if and only if

$$\text{rk } Tf_e(\psi) \leq m.$$  

By imposing these rank conditions to the matrix $Tf_e(\psi)$ we obtain $\binom{3}{2} \binom{2}{2} + 0 + \binom{1}{1} \binom{1}{1} + \binom{2}{2} \binom{1}{1} + \binom{1}{1} \binom{2}{2} = 12$ phylogenetic invariants $\{f_i\}_{i=1,\ldots,12}$:

1. $f_1, \ldots, f_{10}$ have degree 2 and are obtained by the conditions $\text{rk } (S_0), \text{rk } (S_3) = 1$
2. $f_{11}, f_{12}$ have degree one and are obtained by the conditions $S_1, S_4 = 0$. These two invariants are equivalent to Lake’s invariants (cf. [Lak87]).

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