An algebraic analysis of the two state Markov model on tripod trees

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Abstract

Methods of phylogenetic inference use more and more complex models to generate trees from data. However, even simple models and their implications are not fully understood. Here, we investigate the two-state Markov model on a tripod tree, inferring conditions under which a given set of observations gives rise to such a model. This type of investigation has been undertaken before by several scientists from different fields of research.

In contrast to other work we fully analyse the model, presenting conditions under which one can infer a model from the observation or at least get support for the tree-shaped interdependence of the leaves considered.

We also present all conditions under which the results can be extended from tripod trees to quartet trees, a step necessary to reconstruct at least a topology. Apart from finding conditions under which such an extension works we discuss example cases for which such an extension does not work.

Keywords: Phylogenetics, Identifiability, Invariant, Two-State-Model

1. Introduction

In phylogeny, one assumes that the relationship of a set of taxonomic units (or taxa) can be visualised by a (binary) tree. The aim is to derive this tree from the observations at the taxa. From a stochastic modelling point of view, one assigns the taxa to the leaves of a (binary) tree, and assumes that the observations (which are usually considered to be i.i.d. over different sites) are the end results of a Markov process along the tree. The goal is to derive the best combination of tree and Markov model to explain the observations.

This work regards the identifiability problem of this inference. It essentially asks whether it is possible that infinite data sets are able to uniquely identify the transitions on the tree and the tree completely. Note that in the present context, identifiability

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Preprint submitted to Math. Biosci. December 6, 2011
readily leads to consistency of various methods of estimating the parameters of the model [see [1, Section 2.2 for an overview].

However, usually one only has an estimate of the leaf distribution such a process induces. This leads to the question of whether one can find (simple) conditions to determine whether a taxon distribution comes from a Markov process. In other words, we ask whether we can validate the model, at least if there are infinitely many data points available.

To approach this problem, we consider a very simple model. We assume that our process can take only one of two states for every site, and that the tree is a tripod tree.

Under these restrictions, we can completely describe the map from the taxon distribution to the parameters of the model, including necessary and sufficient conditions on positivity of the parameters. Thereby, no conditions for reversibility of the processes on the edges are needed. The analysis of the model on tripod trees has immediate consequences for quartet trees. We derive these conditions to exemplify the shortcomings of an extension from tripods to quartets.

Technically, the generic part of this work is already well-known. Initial work on the two-state model from psychology can be found in Lazarsfeld and Henry [3]. Pearl and Tarsi [4] used these results in artificial intelligence to algorithmically identify the whole tree behind two-state Markov models. Note that identifiability of Markov models especially in phylogeny was studied in Allman et al. [5], Allman and Rhodes [6, 7], Baake [8], Chang [2]. We add to those results the analysis of the degenerate cases, together with a complete analysis of the quartet tree model.

The typical tool (for multi-state models) to identify a subspace of taxon distributions which might come from a Markovian tree model are phylogenetic invariants [6, 7, 9, 10, 11, 12]. Those invariants are polynomials in the taxon distribution which are zero for those distributions that are derived from the model of interest.

Sumner et al. [13] discuss another very interesting set of invariants, the so-called Markov invariants. These are invariants whose value on a tree scales with the determinants of the Markov matrices on the edges. Thus, Markov invariants indicate simple relations between the observations (the distribution of leaf states) and the model (described by the Markov matrices), and provide conditions on the observations based on properties of the model. We will make use of this property in this work.

In the two-state tripod case there is only one, the trivial invariant. But, not all leaf distributions are derived from the Markov model. In fact, we derive polynomials that vanish on distributions which satisfy the trivial invariant but are not identifiable under the Markov model. To accommodate this observation we suggest incorporating these polynomials into the set of invariants but with the addition that these polynomials do not vanish for identifiable distributions. We discuss degenerate distributions to describe this observation.

Although most of the leaf distributions allow for complex solutions of the model equations, in order for the solution of the algebraic equation to be parameters of a Markov model additional inequalities must be fulfilled [15, 16, 17]. The approach of
Matsen is restricted to the Cavender-Farris-Neyman model [CFN 18, 19, 20] to accommodate the Hadamard approach [21, 22]. Yang [17] investigated the CFN model to explore conditions to obtain solutions for different optimisation problems in phylogeny. Extending our approach we recover the inequalities presented in Pearl and Tarsi [4].

As a final step we investigate how the results for tripod trees extend to trees of four leaves. The results provide a glimpse at what we can expect from the reconstruction from tripods when we have no knowledge of the identifiability of the given taxon distribution.

The structure of this work is as follows: In Section 2 we describe the general mutation model on a tree, with specialisation to tripod trees coming in Section 3. Section 4 deals with the complete solution of the two-state tripod tree model. Then, in Section 5 we use these results to analyse the general two-state Markov model on quartet trees. Section 6 discusses the relation between our work and the concept of Markov invariants, and possible extensions of this work. For the sake of readability, proofs are presented in Appendix A.

2. The Markov model of mutation along a tree

In this section we introduce the general Markov model and its properties. Pearl and Tarsi [4] nicely motivate this model in the following way. Assume, one is given a set $L$ of taxa and a set of observations from a Markov process $X : L \rightarrow \{0, 1\}$. From these observations one deduces a correlation between the taxa. The assumption is that this correlation can be explained by an underlying (binary) tree $T = (V, E)$ and an extension $Y : V \rightarrow \{0, 1\}$ of $X$ such that for any pair of taxa there is an interior node such that given the state at the interior node the two taxa are independent. See Fig. [A.1] for a depiction of this.

[Figure 1 about here.]

Let us look closer at the process $Y$. The independence of pairs of taxa given an interior node on the path between them corresponds to the so-called directed local Markov property [e.g., 23, Chapter 2]. For this property one has to identify a node $\zeta \in V$ as the root of the tree and direct all edges away from $\zeta$. Thus, our tree becomes a directed acyclic graph, and for every node $\beta \in V \setminus \{\zeta\}$ there is a parent node $\alpha \in V$ (with respect to the root), such that $(\alpha, \beta) \in E$. Further, for each node $\beta \in V$ one defines the set its descendants as those nodes $\alpha$ for which the path from the root to $\alpha$ passes through $\beta$. The non-descendants are then the nodes that are neither descendants nor parents.

The directed local Markov property states that conditioned on the state of its parent node the state of a node $\alpha \in V$ is independent of the states of its
non-descendants. With this property the joint distribution \( \tilde{p}^Y \) has the factorisation property, i.e. for the joint state \( \chi \in \{0, 1\}^{\vert V \vert} \) we get

\[
\tilde{p}^Y_{\chi} = \Pr[Y_\zeta = \chi_\zeta] \prod_{(\alpha, \beta) \in E} \Pr[Y_\beta = \chi_\beta \mid Y_\alpha = \chi_\alpha] = q^\zeta_{\chi_\zeta} \prod_{(\alpha, \beta) \in E} M^{\alpha\beta}_{\chi_\alpha \chi_\beta}.
\] (1)

Here, the marginal distribution \( q^\zeta \) corresponds to the initialisation of the process, i.e. \( q^\zeta_z \) is the probability that the process attains state \( z \in \{0, 1\} \) at the root. The transition matrices \( (M^e)_{e \in E} \) describe the way the process progresses along an edge. E.g., for an edge \( (\alpha, \beta) \in E \) the term \( M^{\alpha\beta}_{ab} \) is the probability that the character \( a \) at node \( \alpha \) is mutated into character \( b \) at node \( \beta \).

In summary, the joint probability distribution \( \tilde{p}^Y \) is given by the marginal distribution \( q^\zeta \) and the transition matrices \( (M^e)_{e \in E} \), and thus such a Markov process is completely characterised by these parameters. We will call \( q^\zeta \) and \( (M^e)_{e \in E} \) the process parameters.

In general, the actual position of the root node \( \zeta \) is not important for (1), i.e. \( \zeta \) can be chosen arbitrarily from \( V \), including a leaf [e.g., 7].

We only have partial knowledge on the realisations of the process \( Y \) through the process \( X \) on the leaves. The joint distribution \( p^X \) of \( X \) can then be inferred from (1) using the law of total probability. Let \( x \in \{0, 1\}^{\vert L \vert} \) denote the joint state at the leaves. Then

\[
p^X_x = \sum_{\chi \in V} \tilde{p}^Y_{\chi} = \sum_{\chi \in V} q_{\chi_\zeta} \prod_{(\alpha, \beta) \in E} M^{\alpha\beta}_{\chi_\alpha \chi_\beta}.
\] (2)

Note that under the assumption that \( X \) comes from a reversible Markov process \( Y \) Chang [2] proved that all process parameters can be recovered from all the distributions of the restrictions of \( X \) to arbitrary triples of taxa.

If we find process parameters for a joint taxon distribution \( p \) then we call \( p \) tree decomposable. If the obtained process parameters are unique (up to model-specific symmetries), we call \( p \) algebraically identifiable, and if further the process parameters are marginal and transition probabilities, then \( p \) is called stochastically identifiable. Clearly, any stochastically identifiable distribution is also algebraically identifiable.

Looking at (2) we realise that verifying the tree decomposability of a distribution \( p \) is equivalent to solving a polynomial equation system of \( 2^{\vert L \vert} - 1 \) independent equations in \( 4^{\vert L \vert} - 5 \) variables. We observe that the Markov equations are overdetermined for \( \vert L \vert > 3 \), i.e. the space of tree decomposable distributions is a proper subspace of the space of all distributions. From this we conclude, that there are conditions that define a tree decomposable distribution. These conditions are generally known as invariants, polynomials in \( 2^{\vert L \vert} - 1 \) variables whose roots are distributions that are tree decomposable. One example of an invariant is

\[
\sum_{x \in \{0, 1\}^{\vert L \vert}} p_x = 1,
\] (3)
i.e. all probabilities sum to one. This is fittingly called the trivial invariant. Allman and Rhodes [6] provide a complete set of invariants for trees of arbitrary size under a two-state-model, and observe that for complete identification the knowledge of the restrictions to six taxa are necessary.

However, as pointed out in multiple publications [e.g., 4, 16] such invariants are not sufficient to guarantee tree identifiability. In particular, additional inequalities are needed.

Here, we are not only interested in recapturing invariants and inequalities. In addition, we also investigate those distributions that are not algebraically identifiable or not tree decomposable at all to discuss their impact on invariant-based inference.

3. General properties of a Markov model on a tripod tree

The starting point of our analysis is the tripod tree \( T \) with taxa \( \alpha, \beta, \gamma \), interior node \( \zeta \) and edges \((\zeta, \alpha), (\zeta, \beta), (\zeta, \gamma)\) (see Fig. A.2). This is the only labeled topology for three taxa. Hence any inference will be process- and not topology-related. Allman and Rhodes [7] select a taxon as the root for their approach. We will place the root at the interior node for the symmetry this provides in the tree equations.

As stated in the previous section, if the joint distribution \( p \) of \( X_\alpha, X_\beta, X_\gamma \) comes from a Markov process then there are parameters \( q^\zeta, M^\alpha, M^\beta, M^\gamma \) such that the Markov equations (2) are satisfied. On a tripod tree these equations are the tripod equations

\[
p_{abc} = q^\zeta M_a^\alpha M_b^\beta M_c^\gamma + (1 - q^\zeta) M_{0a}^\alpha M_{0b}^\beta M_{0c}^\gamma, \quad a, b, c \in \{0, 1\}.
\]

As before we call \( p \) tree decomposable, if there are parameters, algebraically identifiable, when the parameters are unique (up to some symmetries discussed later), and stochastically identifiable if the parameters are unique and proper marginal and transition probabilities.

The works of Lazarsfeld and Henry [3] and Pearl and Tarsi [4] were mainly interested in inferring conditions under which a triplet distribution is stochastically identifiable. While recovering their results we also investigate tree decomposability and algebraic identifiability in order to describe their impact on invariant-based inference.

For three taxa the only invariant is the trivial invariant. Thus, one could expect that all triplet distributions are tree decomposable. As we will see later, this is not the case. In fact, we will present polynomials whose roots satisfy the trivial invariant but are not tree decomposable.
3.1. Statistics for binary models

Following Pearl and Tarsi [4], we identify the symbols 0 and 1 with their actual integer counterparts. This permits us to introduce a set of terms that are very helpful for later steps of the analysis. We start by introducing the following abbreviations:

\[ \varepsilon_{\alpha\beta\gamma} := \mathbb{E}X_\alpha X_\beta X_\gamma = \Pr[X_\alpha = 1, X_\beta = 1, X_\gamma = 1] = p_{111}, \]
\[ \varepsilon_{\alpha\beta} := \mathbb{E}X_\alpha X_\beta = \Pr[X_\alpha = 1, X_\beta = 1] = p_{11\Sigma} = p_{110} + p_{111}, \]
\[ \varepsilon_{\alpha} := \mathbb{E}X_\alpha = \Pr[X_\alpha = 1] = p_{1\Sigma\Sigma} = p_{100} + p_{101} + p_{110} + p_{111}. \]

The symbols \( p_{11\Sigma} \) and its modifications \( p_{1\Sigma1} \) etc. are direct consequences of the application of the law of total probability to the equation system (4). These terms are also known as *marginalisations* leading to a removal of a random variable from consideration by summing over its states. This linear modification means we can study the tripod equations (4) also in terms of its marginalisations.

In the case of the binary model the above symbols \( \varepsilon_A \) for all \( A \in L \) correspond to the joint mean of the random variables for the taxa in \( A \). Using these definitions we can introduce simple terms which correspond to the covariances between the set of random variables:

\[ \tau_{\alpha\beta} := \text{Cov}[X_\alpha, X_\beta] = \mathbb{E}X_\alpha X_\beta - \mathbb{E}X_\alpha \mathbb{E}X_\beta, \]

with equivalent definitions for \( \tau_{\alpha\gamma} \) and \( \tau_{\beta\gamma} \). Of further interest are the following terms \((c \in \{0, 1\})\)

\[ \tau_{\alpha\beta|c} := p_{11c}p_{\Sigma\Sigma c} - p_{1\Sigma c}p_{\Sigma1 c}, \]

with equivalent definitions for \( \tau_{\alpha\gamma|b}, b \in \{0, 1\} \) and \( \tau_{\beta\gamma|a}, a \in \{0, 1\} \). These terms are actually multiples of the conditional covariances, \( \text{Cov}[X_\alpha, X_\beta|X_\gamma = c] = \tau_{\alpha\beta|c}/p_{\Sigma\Sigma c} \).

Finally, we also introduce the three-way covariances

\[ \tau_{\alpha\beta\gamma} := \text{Cov}[X_\alpha, X_\beta, X_\gamma] = \mathbb{E}(X_\alpha - \mathbb{E}X_\alpha)(X_\beta - \mathbb{E}X_\beta)(X_\gamma - \mathbb{E}X_\gamma) \]
\[ = \varepsilon_{\alpha\beta\gamma} - \varepsilon_{\alpha}\varepsilon_{\beta\gamma} - \varepsilon_{\beta}\varepsilon_{\alpha\gamma} - \varepsilon_{\gamma}\varepsilon_{\alpha\beta} + 2\varepsilon_{\alpha}\varepsilon_{\beta}\varepsilon_{\gamma}. \]

For a review on covariance for more than two random variables see e.g. Rayner and Beh [24]. The term \( \tau_{\alpha\beta\gamma} \) describes the interactions of the three leaves considered. Sumner et al. [13] call this term a *stangle*, a stochastic tangle, highlighting its relation to entangled states of qbits in quantum mechanics. The three-way covariances are zero in the case of symmetric models like CFN, which also reflects the findings in Baake [8]. However, for more complex models the three-way covariances are needed as indicated by the findings of Chang [2].

Since covariances are a measure of interdependence of random variables, and because the identification of a tree and a Markov model is an interpretation of the interdependence in terms of hidden variables and conditional independence, looking at these covariances is a very logical way to verify whether or not such an interpretation is admissible. Using these terms we can immediately propose a useful property.
Lemma 1. Let $p$ denote the joint probability for binary random variables $X_\alpha$, $X_\beta$ and $X_\gamma$. If we flip the state in one taxon, then we flip the signs in its pairwise covariances. E.g., if $X_\alpha \mapsto 1 - X_\alpha$, then $\tau_{\alpha \beta} \mapsto -\tau_{\alpha \beta}$, $\tau_{\alpha \gamma} \mapsto -\tau_{\alpha \gamma}$, $\tau_{\beta \gamma} \mapsto \tau_{\beta \gamma}$.

One immediate consequence of this observation is that the product $\tau_{\alpha \beta} \tau_{\alpha \gamma} \tau_{\beta \gamma}$ always has the same sign no matter how much we flip states.

3.2. Tree properties

In this section we assume that $p$ is tree decomposable and regard some immediate consequences. We will later see that these conditions are necessary for identifiability but not sufficient. Nevertheless, these conditions provide some immediate insights for it.

Lemma 2.
1. If a triplet distribution $p$ is tree decomposable on $T$ with $\tau_{\alpha \beta} = 0$, then also $\tau_{\alpha \beta \gamma} = 0$ and $\tau_{\alpha \gamma} = 0$ or $\tau_{\beta \gamma} = 0$.
2. If a triplet distribution $p$ is stochastically identifiable then the product $\tau_{\alpha \beta} \tau_{\alpha \gamma} \tau_{\beta \gamma}$ is non-negative.

The non-negativity of the product has already been verified by Lazarsfeld and Henry [3]. With Lemma 1, it is not complicated to derive that on a star tree (with arbitrary number of leaves) there always is a state flipping such that all pairs of leaves are positively correlated.

Corollary 3. Suppose we are given a stochastically identifiable distribution $p$ on a tree with finite leaf set $L$ such that the pairwise covariances do not vanish, i.e., $\tau_{\alpha \beta} \neq 0$ for all $\alpha, \beta \in L$. Then there exists a set of leaves $L_0 \subset L$ such that flipping the states of the leaves in $L_0$ yields all covariances $\tau_{\alpha \beta}$, $\alpha, \beta \in L$, being positive.

Lemma 2(1) occurs exactly if $X_\alpha$ or $X_\beta$ is independent of the remaining random variables. It also implies the following:

Corollary 4. A triplet distribution $p$ with $\tau_{\alpha \beta} = 0$ but $\tau_{\alpha \gamma} \neq 0$ and $\tau_{\beta \gamma} \neq 0$ is not tree decomposable.

Thus we already see, that the trivial invariant does not characterise tree decomposable distributions in this setting. The following example shows that such cases can be easily constructed.

Example 1. Triplet distributions of type

$$p = (p_{000}, p_{001}, p_{010}, p_{011}, p_{100}, p_{101}, p_{110}, p_{111}) = (4 - x, x, 2, 2, 2, 2, 2, 2)/16, \quad x \in [0, 4] \setminus \{2\},$$

yield $\tau_{\alpha \beta} = 0$ but $\tau_{\alpha \gamma} = \tau_{\beta \gamma} = (2 - x)/32$ and hence are not tree decomposable. In fact, for binary variables a much more complicated graphical model with more “inner” nodes and edges is needed to explain these covariances.
4. Solving the tripod equations

In this section we are given a triplet distribution $p$ and infer conditions under which it is algebraically identifiable. For each case we will present an example.

4.1. The algebraic solution

As has been pointed out multiple times, the only invariant in the tripod case is the trivial invariant. In other words, the “set” of invariants for a tripod tree is satisfied by all triplet distributions. However, as we have seen in Corollary 4 there are triplet distributions that are not tree decomposable even though they satisfy the trivial invariant. Thus executing the actual decomposition, i.e. finding a solution for the tripod equations not only provides complete forms for the parameters but is also helpful to identify further cases. The first task is to clarify up to which level of uniqueness the decomposition of a triplet distribution can be attained. To do this we look at the implications of a state-flip at the root.

**Lemma 5.** If a triplet distribution $p$ is tree decomposable with parameters $q^ζ, M^α, M^β, M^γ$ then it is also tree decomposable for parameters $\tilde{q}^ζ, \tilde{M}^α, \tilde{M}^β, \tilde{M}^γ$ with

$$\tilde{q}^ζ = q^{ζ}_1 - z, \quad \tilde{M}^α = M^α(1 - z)a, \quad \tilde{M}^β = M^β(1 - z)b, \quad \tilde{M}^γ = M^γ(1 - z)c.$$ 

Hence, except for the case where everything is equal to $1/2$, there will always be at least two sets of parameters that decompose a triplet distribution $p$. In terms of molecular evolution one can view these solutions as having either few mutations $(M^δ_{zz} < M^δ_{z(1-z)}, \delta \text{ leaf})$ or many mutations $(M^δ_{z(1-z)} > M^δ_{zz}, \delta \text{ leaf})$ for the other. Chang [2] addressed the problem of symmetric solutions by introducing matrix categories that are reconstructible from rows. One such class consists of diagonally dominant matrices, i.e. $M^α_{zz} > M^δ_{z(1-z)}$ for all leaves and $z \in \{0, 1\}$. If only these two sets of parameters exist then we will regard the associated distribution as algebraically identifiable. It should be noted that the set of symmetric solutions increases with the number of parameters, i.e. each possible permutation of the states at the root yields a new solution. This fact has also been observed by Chang [2] in the case of the time-continuous Markov model.

Next, we present conditions under which $p$ is algebraically identifiable and present the closed form for the parameters.

**Theorem 6.** Let $p$ denote a triplet distribution and assume

$$τ_{αβγ} τ_{αγβ} τ_{βγα} \neq 0, \quad τ_{αβγ} τ_{αγβ} τ_{βγα} \neq -\left(\frac{τ_{αβγ}}{2}\right)^2. \quad (5)$$

Then $p$ is algebraically identifiable. The associated parameters have the following form:

$$q^ζ = \frac{1}{2} - \frac{τ_{αβγ}}{2\sqrt{χ}}, \quad M^α_{01} = ε_α + \frac{τ_{αβγ} - \sqrt{χ}}{2τ_{αγ}}, \quad M^β_{01} = ε_β + \frac{τ_{αβγ} - \sqrt{χ}}{2τ_{αγ}}, \quad M^γ_{01} = ε_γ + \frac{τ_{αβγ} - \sqrt{χ}}{2τ_{αβ}},$$

$$M^α_{11} = ε_α + \frac{τ_{αβγ} + \sqrt{χ}}{2τ_{βγ}}, \quad M^β_{11} = ε_β + \frac{τ_{αβγ} + \sqrt{χ}}{2τ_{αγ}}, \quad M^γ_{11} = ε_γ + \frac{τ_{αβγ} + \sqrt{χ}}{2τ_{αβ}}, \quad (6)$$
where \( \chi = \tau_{\alpha\beta\gamma}^2 + 4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} \).

Note that Pearl and Tarsi [4] presented a similar solution for the parameters.

Looking at the parameters in (6) we see that algebraically the conditions in (5) prevent division by zero. Together with the trivial invariant we can thus claim that the space of algebraically identifiable triplet distributions is given by \( S \setminus (S_0 \cup S_1) \) with

\[
S := \{ p \in \mathbb{R}^8_{+} : p_{000} + \cdots + p_{111} = 1 \},
S_0 := \{ p \in S : \tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} = 0 \},
S_1 := \{ p \in S : \tau_{\alpha\beta\gamma}^2 + 4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} = 0 \}.
\]

Considering (5) and Lemma 2(2) we see that triplet distributions with \( \tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} < 0 \) are only algebraically, but not stochastically identifiable. In fact, for \( -\tau_{\alpha\beta\gamma}^2 < 4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} < 0 \) we get real-valued parameters, and for \( 4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} < -\tau_{\alpha\beta\gamma}^2 \) we get a set of complex-valued parameters.

The following example presents such distributions.

**Example 2.** Regard the distributions

\[
p_1 = (6, 7, 2, 1, 1, 1, 4, 5)/27, \quad p_2 = (6, 7, 1, 2, 1, 1, 4, 5)/27, \quad p_3 = (6, 6, 2, 1, 1, 1, 4, 5)/27.
\]

All three distributions satisfy the conditions (5), i.e. they are algebraically identifiable. For \( p_1 \) the covariance \( \tau_{\beta\gamma} \) is negative and the other two positive, while for \( p_2 \) we have \( \tau_{\alpha\gamma} \) negative and the other two positive. The distribution \( p_3 \) has only positive pairwise covariances.

The parameters for \( p_1 \) are real-valued, the parameters for \( p_2 \) are complex-valued and \( p_3 \) is stochastically identifiable.

Though this example is artificial it indicates just how sensitive the model is to misreads in alignments. E.g., the difference between \( p_1 \) and \( p_3 \) could be seen as reading the pattern 011 under \( p_3 \) as pattern 001 under \( p_1 \).

### 4.2. Stochastically identifiable distributions

The next step is to determine conditions under which a distribution satisfying (5) is stochastically identifiable. These conditions should correspond to the conditions given by Pearl and Tarsi [4, Theorem 1].

Example 2 dealt with \( \tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} < 0 \). However, as the following example shows, positivity of the product does not necessarily yield stochastic identifiability.

**Example 3.** The tripod distribution

\[
p = (68, 0, 20, 12, 20, 12, 17, 51)/200
\]
yields positive covariances for all three pairs but also \( M_{01}^\gamma = -1/20 \), i.e. not a probability.
The example contains a pattern of expected zero occurrence. From the tripod equations we conclude that a stochastically identifiable distribution is strictly positive, thus this example is slightly contrived. However, as Example 1 showed, a strictly positive triplet distribution is not necessarily stochastically identifiable either.

In order to get necessary and sufficient conditions on a triplet distribution to be stochastically identifiable we need to go back to the parameters in (6) and bound them accordingly. This yields:

**Theorem 7.** A triplet distribution \( p \) is stochastically identifiable if and only if after suitable state flips the following inequalities hold

\[
\tau_{\alpha\beta} > 0, \quad \tau_{\alpha\beta|0} \geq 0, \quad \tau_{\alpha\beta|1} \geq 0,
\]

\[
\tau_{\alpha\gamma} > 0, \quad \tau_{\alpha\gamma|0} \geq 0, \quad \tau_{\alpha\gamma|1} \geq 0,
\]

\[
\tau_{\beta\gamma} > 0, \quad \tau_{\beta\gamma|0} \geq 0, \quad \tau_{\beta\gamma|1} \geq 0.
\]

(7)

In other words, the direction of the correlation between a pair of leaves shall not be influenced by the third leaf. With this we can summarise that a triplet distribution is stochastically identifiable if it is in \( S \setminus (S_0 \cup S_1) \) and there is a state flip such that (7) is satisfied.

**Example 4.** The tripod distribution \( p \) from Example 3 has positive pairwise and conditional covariances except for \( \tau_{\alpha\beta|1} = -9/2500 \). Thus it does not satisfy (7).

### 4.3. Non-identifiable cases

The above considerations dealt with cases where a given triplet distribution \( p \) is algebraically identifiable. The final step of the tripod analysis is to regard those distributions that violate the conditions (5). Corollary 4 already discussed the case where one pairwise covariance is zero while the other two are not and we found that they were not tree decomposable. In the following we look at the remaining cases.

**Proposition 8.** Assume that a triplet distribution \( p \) obeys \( \tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} = - (\tau_{\alpha\beta\gamma}/2)^2 \) but \( \tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \neq 0 \). Then \( p \) is not tree decomposable.

In other words, we found another set of triplet distributions that are not tree decomposable.

**Example 5.** The distribution

\[
p = (16, 5, 8, 15, 14, 5, 2, 15)/80
\]

yields \( \tau_{\alpha\beta} = -1/80, \tau_{\alpha\gamma} = 1/40 \) and \( \tau_{\beta\gamma} = 1/8 \) but \( \chi = 0 \) and hence has no factorisation in the sense of (4). As in Example 1 we point out here that there seems to be no simple graphical structure which explains the observed covariances adequately. On the other hand, similarly to Example 2 the simple act of moving 1/80 from pattern 100 to pattern 110 yields algebraic identifiability. This indicates the level of care required when inferring meaning from observed covariances.
Together with Corollary 4 this covers the distributions that are not tree decomposable. The remaining cases are triplet distributions that are tree decomposable but not algebraically identifiable.

**Proposition 9.** Let \( p \) be a triplet distribution with \( \tau_{\alpha\beta} = 0 \) and \( \tau_{\alpha\gamma} = 0 \). Then \( p \) is tree decomposable with infinitely many parameter sets.

The parameter sets are identified by one of the following compositions:

(i) \( \tau_{\beta\gamma} \neq 0 \). Then \( M_{0a}^\alpha = M_{1a}^\alpha = p_{a\Sigma\Sigma}, a \in \{0, 1\} \), and for any \( u, b, c \in \{0, 1\} \):

\[
q_1^\xi = \frac{p_{\Sigma\Sigma} - M_{0c}^\gamma}{M_{0c}^\gamma - M_{1c}^\gamma}, \quad M_{ab}^{\beta} = \frac{p_{\Sigma\Sigma} - p_{\Sigma\Sigma}M_{(1-u)c}^{\gamma}}{p_{\Sigma\Sigma} - M_{(1-u)c}^{\gamma}}
\]

with free parameters \( M_{0c}^\gamma \neq M_{1c}^\gamma \).

(ii) \( \tau_{\beta\gamma} = 0 \). Then for all \( a, b, c, \in \{0, 1\} \) the free parameters can be distributed as follows:

(a) \( M_{0a}^\alpha = M_{1a}^\alpha = p_{a\Sigma\Sigma}, M_{0b}^\beta = M_{1b}^\beta = p_{\Sigma\Sigma} \) and

\[
q_1^\xi = \frac{p_{\Sigma\Sigma} - M_{0c}^\gamma}{M_{1c}^\gamma - M_{0c}^\gamma},
\]

with free parameters \( M_{0c}^\gamma \neq M_{1c}^\gamma \).

(b) \( M_{0a}^\alpha = M_{1a}^\alpha = p_{a\Sigma\Sigma}, M_{0b}^\beta = M_{1b}^\beta = p_{\Sigma\Sigma}, M_{0c}^\gamma = M_{1c}^\gamma = p_{\Sigma\Sigma} \) with free parameter \( q_1^\xi \).

(c) \( q_1^\xi = 0, M_{0a}^\alpha = p_{a\Sigma\Sigma}, M_{0b}^\beta = p_{\Sigma\Sigma}, M_{0c}^\gamma = p_{\Sigma\Sigma} \) with free parameters

\( M_{1a}^\alpha, M_{1b}^\beta, M_{1c}^\gamma \).

In other words, the distribution is tree decomposable because process parameters exist but it is not algebraically identifiable because we have no means to recover the true parameters or more precisely, there are infinitely many parameters that yield the same distribution.

**Example 6.** The triplet distribution

\[
p = (2, 2, 2, 2, 2, 2, 2)/16
\]

yields complete independence of the leaves \( \tau_{\alpha\beta} = \tau_{\alpha\gamma} = \tau_{\beta\gamma} = 0 \), i.e. the case (ii) in Proposition 9 is to be regarded here. It is not too surprising that such a distribution yields an infinite number of solutions since the state at the root is completely undetermined.

Looking again at the cases listed above, we see that \( X_\alpha \) is not only pairwise independent from \( (X_\beta, X_\gamma) \) (induced by \( \tau_{\alpha\beta} = \tau_{\alpha\gamma} = 0 \)), but even completely independent. Then the multiple solutions come from the fact that we can place the root arbitrarily between \( \beta \) and \( \gamma \).

The good news is, that the non-identifiable cases form a small subset among all triplet distributions. In fact:
Proposition 10. Non-identifiable triplet distributions, i.e. distributions violating the conditions \[5\] form a Lebesgue zero set in the set of all possible triplet distributions.

This concludes our analysis of the tripod case. We identified the subset of triplet distributions that are uniquely algebraically and stochastically identifiable, and those that are tree decomposable but not algebraically identifiable, or not tree decomposable at all.

5. Extension to quartet trees

In this section we will explore the implications of extending the results for three taxa to four taxa. For this section we look at the quartet tree \( Q = (V,E) \) with

\[ V = \{\zeta,\psi,\alpha,\beta,\gamma,\delta\}, \quad E = \{(\zeta,\psi), (\zeta,\alpha), (\zeta,\beta), (\psi,\gamma), (\psi,\delta)\}. \]

Fig. A.3 provides an illustration including the four tripod restrictions

\[ T = T_{\alpha\beta\gamma}, \quad \tilde{T} = T_{\alpha\beta\delta}, \quad \hat{T} = T_{\alpha\gamma\delta} \quad \text{and} \quad \check{T} = T_{\beta\gamma\delta}. \]

Regard the quartet distribution \( \pi = (\pi_{abcd})_{a,b,c,d \in \{0,1\}} \) describing the joint distribution for \( \alpha, \beta, \gamma \) and \( \delta \). If \( \pi \) is stochastically identifiable and reversible then it can be reconstructed from the marginalisations on its four tripods \[2\], i.e. computing the parameters for all tripods will immediately return the full process. However, the converse is not necessarily true. As Example \[7\] below shows, there are cases where each tripod marginalisation is stochastically identifiable but no quartet tree can be reconstructed.

[Figure 3 about here.]

Pearl and Tarsi \[4\] presented an algorithm to reconstruct the topology for an arbitrary number of taxa. Their algorithm employs the condition that tripods that share an interior node in the (unknown) tree topology must have the same marginal distribution at this interior node. Their approach yields an invariant, which for \( Q \) amounts to

\[ f_1(\pi) = \tau_{\alpha\delta}\tau_{\beta\gamma} - \tau_{\alpha\gamma}\tau_{\beta\delta}. \]

This invariant is related to the four-point-condition [e.g., \[26\], p. 146] and thus topologically informative, i.e. it is particular to topology \( Q \). If a distribution \( \pi \) is from another tree than \( f_1(\pi) \neq 0 \).

To reconstruct the process parameters as well, more invariants are needed. In particular, for \( \pi \) to be algebraically identifiable on \( Q \) the parameters obtained from the tripod marginalisations must satisfy the following properties:

1. The parameters for edges \( (\zeta,\alpha) \), \( (\zeta,\beta) \) and \( q^\zeta \) obtained from triplet distributions \( \bar{p} \) and \( \tilde{p} \), respectively, must be equal.

2. The parameters for edges \( (\psi,\gamma) \), \( (\psi,\delta) \) and \( q^\psi \) obtained from triplet distributions \( \hat{p} \) and \( \check{p} \), respectively, must be equal.
3. The parameters $M^\psi$ for the interior edge $(\zeta, \psi)$ are obtained from the equations

$$\begin{align*}
\bar{M}^\gamma_{01} &= (1 - M^\psi_{01})\bar{M}^\gamma_{01} + M^\psi_{01}\bar{M}^\gamma_{11}, \\
\bar{M}^\gamma_{11} &= (1 - M^\psi_{11})\bar{M}^\gamma_{01} + M^\psi_{11}\bar{M}^\gamma_{11}.
\end{align*}$$

(11)

These equations must hold equivalently when $\gamma$ is replaced by $\delta$ and the parameters come from tripod $\bar{T}$ instead of $\bar{M}$.

These conditions imply further restrictions on $\pi$. An indicator for the minimal number of such conditions is the observation that a quartet distribution $\pi$ has 15 degrees of freedom, but there are only 11 process parameters on $Q$, two for each edge and one for the root distribution. Thus we need at least four additional conditions or rather invariants. We will use the above observations to derive an equivalent set of invariants.

**Proposition 11.** A quartet distribution $\pi$ is algebraically identifiable on $Q$ if its tripod marginalisations satisfy conditions (5) and the following invariants vanish on $\pi$:

$$\begin{align*}
f_0(\pi) &= \epsilon_{\alpha\beta\gamma}\Lambda_{\alpha\gamma} - \epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\gamma}\delta + \epsilon_{\gamma}\epsilon_{\alpha\beta}\epsilon_{\alpha\gamma}\delta + \epsilon_{\alpha}\epsilon_{\gamma}\delta\epsilon_{\alpha\beta}\epsilon_{\alpha\gamma}\delta - \epsilon_{\alpha\beta}\epsilon_{\alpha\gamma}\epsilon_{\gamma}\delta, \\
f_1(\pi) &= \tau_{\alpha}\delta\tau_{\beta}\gamma - \tau_{\alpha}\gamma\tau_{\beta}\delta, \\
f_2(\pi) &= \tau_{\alpha}\gamma\tau_{\beta}\gamma\delta - \tau_{\alpha}\beta\gamma\tau_{\alpha}\gamma\delta, \\
f_3(\pi) &= \tau_{\alpha}\gamma\tau_{\alpha}\beta\delta - \tau_{\alpha}\beta\gamma\tau_{\alpha}\delta.
\end{align*}$$

The parameters unique up to state flip at the interior nodes are then given by Theorem 6 and

$$\begin{align*}
M^\psi_{01} &= \frac{1}{2} + \frac{\tau_{\alpha}\delta\tau_{\alpha}\beta\gamma - \tau_{\alpha}\beta\tau_{\alpha}\gamma\delta - \tau_{\alpha}\delta\sqrt{\chi_{\alpha\beta\gamma}}}{2\tau_{\alpha}\beta\sqrt{\chi_{\alpha\beta\delta}}}, \\
M^\psi_{11} &= \frac{1}{2} + \frac{\tau_{\alpha}\delta\tau_{\alpha}\beta\gamma - \tau_{\alpha}\beta\tau_{\alpha}\gamma\delta + \tau_{\alpha}\delta\sqrt{\chi_{\alpha\beta\gamma}}}{2\tau_{\alpha}\beta\sqrt{\chi_{\alpha\beta\delta}}}.
\end{align*}$$

(12)

The existence of these invariants means that tree decomposable quartet distributions form a Lebesgue zero set in the set of all quartet distributions for the same reason that the non-identifiable sets are a Lebesgue zero set in the set of all tree decomposable distributions.

Invariant $f_1$ comes from the equality of the marginal distributions at the interior nodes, as proposed by Pearl and Tarsi [4]. Invariants $f_2$ and $f_3$ come from the equality of edge transition matrices. Hence, distributions for which $f_1$, $f_2$ and $f_3$ vanish will uniquely identify topology $Q$. Therefore, $f_1$ to $f_3$ are topologically informative.

However, only distributions for which $f_0$ vanishes will be subject to the inferred parameters. In other words, in the set of zero points for $f_1$ to $f_3$ there is a set of distributions that returns the same set of parameters for $Q$, but only for one of these distributions $f_0$ vanishes. It would be interesting to investigate how this distribution
relates to the set it projects from, e.g. if it is related to the possible maximum likelihood optimum.

Despite the fact that $f_1$ to $f_3$ are sufficient to infer a topology, $f_0$ is also topologically informative in that it will not vanish for distributions coming from another tree.

In the case of the CFN model, all triplet covariances vanish. Hence, only invariants $f_0$ and $f_1$ are of interest in that case. Therefore, either invariant is sufficient to identify the associated tree topology.

The parameters for the interior edge do not add more non-identifiable cases. However, as in the tripod case, further conditions are needed to guarantee quartet identifiability.

**Proposition 12.** A quartet distribution is stochastically identifiable if and only if every triplet marginalisations satisfies both Theorem 7 and the following inequalities

$$
\tau_{\alpha\delta}\sqrt{X_{\alpha\beta\gamma}} - \tau_{\alpha\beta}\sqrt{X_{\alpha\gamma\delta}} \leq \tau_{\alpha\beta}\tau_{\alpha\gamma}\delta - \tau_{\alpha\delta}\tau_{\alpha\beta}\gamma \leq \tau_{\alpha\beta}\sqrt{X_{\alpha\gamma\delta}} - \tau_{\alpha\delta}\sqrt{X_{\alpha\beta\gamma}}.
$$

(13)

All other relations are covered due to the fact that the quartet distribution $p$ needs to satisfy the invariants $f_0 - f_3$. The following example provides a very nice case in which reconstruction is not possible but offers a very interesting challenge.

**Example 7.** Chor et al. [27] discussed several examples of distributions with multiple maxima of the likelihood function. These examples relate to the CFN model, i.e., $p_{abcd} = p(1-a)(1-b)(1-c)(1-d)$ so that the Hadamard approach can be used. Regard the symmetric distribution

$$p = (14, 0, 0, 3, 0, 2, 1, 0, 0, 1, 2, 0, 3, 0, 0, 14)/40. \quad (14)$$

Retrieving the statistics yields:

$$\tau_{\alpha\beta} = 7/40 = \tau_{\gamma\delta}, \quad \tau_{\alpha\gamma} = 3/20 = \tau_{\beta\delta}, \quad \tau_{\alpha\delta} = 1/8 = \tau_{\beta\gamma},$$

$$\tau_{\alpha\beta}\gamma = \tau_{\alpha\beta}\delta = \tau_{\alpha\gamma}\delta = \tau_{\beta\gamma}\delta = 0.$$

The last equality immediately shows, that the above distribution will trivially satisfy invariants $f_2$ and $f_3$. However, we get $f_1 = -11/1600$ and $f_0 = -23/375$, i.e. our observations do not come from the quartet tree defined by the bipartition $\alpha\beta|\gamma\delta$.

Looking at the alternative invariants for $f_1$, i.e. at

$$f_1^{\alpha\delta\beta\gamma} = \tau_{\alpha\beta}\tau_{\gamma\delta} - \tau_{\alpha\gamma}\tau_{\beta\delta} = 13/1600,$$

$$f_1^{\alpha\gamma\beta\delta} = \tau_{\alpha\beta}\tau_{\gamma\delta} - \tau_{\alpha\delta}\tau_{\beta\gamma} = 3/200,$$

we see that this distribution comes from none of the available quartet trees.

Nevertheless, we shall have a look at the parameters. Note that the symmetry of the distribution $p$ implies $M_{01}^\alpha = 1 - M_{11}^\alpha =: \overline{M}_\alpha$. Looking at the numerical values for the parameters for every tripod tree we find surprising similarities:
These parameters permit us to infer parameters $M_\zeta = 1/14$ and $M_\psi = 1/7$ such that e.g. the parameters for $\alpha$ on the tripod trees $\alpha\beta\delta$ and $\alpha\gamma\delta$ can be obtained from the parameter for tripod tree $\alpha\beta\gamma$ by

$\tilde{M}_\alpha = M_\zeta(1 - M_\alpha) + (1 - M_\zeta)M_\alpha,$  
$\tilde{M}_\alpha = M_\psi(1 - M_\alpha) + (1 - M_\psi)M_\alpha,$

with analogue assignments for the other leaves. These computations can be visualised by the network in Fig. A.4. The assignment of probabilities for each split permits to justify the observations for each of the four tripod trees. However, the visualisation is misleading because the factorisation of the system does not follow the edges in the network [e.g., ? ? 28].

6. The connection with Markov invariants

This section investigates the connection between the work presented here and the concept of Markov invariants as coined by Sumner et al. [13]. To show these relations we will look back at our covariances and investigate their relationship with the parameters.

Following Allman and Rhodes [6] one can write the three-way-probabilities as a $2 \times 2 \times 2$ tensor $P^{\alpha\beta\gamma}$ such that

$P^{\alpha\beta|0} = \begin{pmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{pmatrix}, \quad P^{\alpha\beta|1} = \begin{pmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{pmatrix}.$

With this as a basis we easily infer our pairwise covariances in terms of determinants of dimensional restrictions of $P^{\alpha\beta\gamma}$. E.g., a marginalisation over $\gamma$ corresponds to $P^{\alpha\beta\Sigma} = P^{\alpha\beta|0} + P^{\alpha\beta|1}$. The determinant of this matrix then corresponds to

$\det P^{\alpha\beta\Sigma} = p_{00}\Sigma p_{11}\Sigma - p_{01}\Sigma p_{10}\Sigma$
$= p_{11}\Sigma(p_{00}\Sigma + p_{11}\Sigma + p_{01}\Sigma + p_{10}\Sigma) - (p_{10}\Sigma + p_{11}\Sigma)(p_{01}\Sigma + p_{11}\Sigma)$
$= p_{11}\Sigma - p_{11}\Sigma p_{11}\Sigma = \tau_{\alpha\beta}.$

Thus, we have invariably obtained an alternative way to compute the covariances. In a similar fashion, if we take the determinant of the conditional kernels $P^{\alpha\beta|c}, c \in \{0, 1\}$, we arrive at the (not normalised) conditional covariance $\tau_{\alpha\beta|c}$:

$\det P^{\alpha\beta|c} = p_{00c}p_{11c} - p_{01c}p_{10c}$
$= p_{11c}(p_{00c} + p_{11c} + p_{01c} + p_{10c}) - (p_{10c} + p_{11c})(p_{01c} + p_{11c})$
$= p_{11c}p_{11c} = \tau_{\alpha\beta|c}.$
It must be noted that the determinant has been used earlier in connection with LogDet families [e.g., 25]. In order to relate these findings to the process parameter, let us
denote by $\Pi = \text{diag}(q^\zeta)$ the diagonal matrix of the marginal distribution at the root,
and with

$$M^\alpha = \begin{pmatrix} M^\alpha_{00} & M^\alpha_{01} \\ M^\alpha_{10} & M^\alpha_{11} \end{pmatrix}$$

the transition matrix for leaf $\alpha$. Then the marginalisation of Equation (2) can be
written as

$$P^\alpha_{\beta \Sigma} = (M^\alpha)^{T} \Pi M^\beta,$$

(15)

where $\Pi$ is the marginal distribution at the most recent common ancestor of $\alpha$ and $\beta$.

If $E_{\alpha\beta}$ is defined as the set of edges connecting the root of the tree and the most recent
common ancestor of $\alpha$ and $\beta$ then we compute $\Pi$ by

$$\Pi = \Pi \prod_{e \in E_{\alpha\beta}} M^e.$$

If we take the determinant on both sides of Eq. (15) we get

$$\det P^\alpha_{\beta \Sigma} = \det M^\alpha \det M^\beta \det \Pi \prod_{e \in E_{\alpha\beta}} \det M^e.$$

We further observe that the determinant in the two-state-case is equal to

$$\det M^\alpha = 1 - M^\alpha_{00} - M^\alpha_{11} = -(M^\alpha_{11} - M^\alpha_{01}).$$

Going back to a tripod tree under the two-state-model this yields the relation

$$\tau_{\alpha\beta} = (M^\alpha_{11} - M^\alpha_{01})(M^\beta_{11} - M^\beta_{01}) q^\zeta_1 (1 - q^\zeta_1).$$

(16)

This relation has been observed in Steel [25] and forms the basis for LogDet inference.
The covariances $\tau_{\alpha\beta}$ also form the simplest form of Markov invariants. Sumner et al.
[13] define these terms in general by:

$$f(p) = g(\hat{p}) \prod_{e \in E} (\det M^e)^{k_e},$$

(17)

with $k_e \in \mathbb{Z}$ denoting the exponent for edge $e \in E$. The term $g(\hat{p})$ describes a function
depicting the relationship of a reduced structure in the tree. Sumner et al. [13] give one
example of such a reduced structure as the tree for which the pendant edges have been
reduced to length zero. In the case of the tripod tree this reduced structure corresponds
to the interior node $\zeta$, and hence the distribution $\hat{p}$ is equivalent to $q^\zeta$ only. In this
setting, Markov invariants are one-dimensional “representations” of the stochastic
models used for inference, such that the complex structure of these models is retained [14].

In our framework, we rediscover more Markov invariants of type (17) when investigating how the remaining covariances are related to the process parameters under the tripod equations (4). In fact, we find:

\[ \tau_{\alpha \beta \gamma} = (M_{11}^{\alpha} - M_{01}^{\alpha})(M_{11}^{\beta} - M_{01}^{\beta})(M_{11}^{\gamma} - M_{01}^{\gamma})q_1^1(1 - q_1^1)(1 - 2q_1^1), \]  

(18)

\[ \tau_{\alpha \beta \gamma} \tau_{\alpha \gamma \beta} = (M_{11}^{\alpha} - M_{01}^{\alpha})^2(M_{11}^{\beta} - M_{01}^{\beta})^2(M_{11}^{\gamma} - M_{01}^{\gamma})^2(q_1^1)^3(1 - q_1^1)^3, \]  

(19)

\[ \chi = (M_{11}^{\alpha} - M_{01}^{\alpha})^2(M_{11}^{\beta} - M_{01}^{\beta})^2(M_{11}^{\gamma} - M_{01}^{\gamma})^2(q_1^1)^2(1 - q_1^1)^2. \]  

(20)

with equivalent terms for the other covariances. These equivalences permit a different way to prove Theorem 6 from the one we present in Appendix A.

It should be noted that our interpretation of the above Markov invariants as covariances only works for the two state model. On the other hand, the form of the Markov invariants stays valid, even though they might not be as immediately apparent from the model as in the cases discussed here. However, in the case of the two-state model using the notion of covariance permits a good interpretation of the findings.

We observe for the (not normalised) conditional covariances

\[ \tau_{\alpha \beta \gamma|c} = (M_{11}^{\alpha} - M_{01}^{\alpha})(M_{11}^{\beta} - M_{01}^{\beta})M_{00}^{\gamma}M_{10}^{\gamma}q_1^1(1 - q_1^1), \]  

(21)

i.e., the transition matrix for leaf \( \gamma \) shall be included into the term \( g(\hat{p}) \) for (17) to be valid. On the other hand, remember that we did not use these covariances to solve the tripod equations (4). We need them only to formulate the positivity constraints in Theorem 7. This property is beyond the purely algebraic framework.

In summary, Markov invariants are very useful when investigating properties of and conditions on leaf distributions \( p \). Especially, they explore the relationship of process parameters and leaf distribution such that phylogenetic invariants like \( f_1 \) to \( f_3 \) from Proposition 11 can be easily extracted. We will employ these relationships to prove the results of Section 3.

7. Discussion

Acknowledgements. We thank Elizabeth S. Allman and John A. Rhodes for stimulating the finalization of the manuscript as well as for sharing their thoughts on this subject with us. Further, we owe much to the discussions with David Bryant, Mike Steel, and Arndt von Haeseler. Suggestions from Jessica Leigh and three anonymous referees are greatly appreciated.

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Appendix A. Proofs

Proof of Lemma 1. A state flip replaces the probabilities at leaf $\alpha$ implies a “new” distribution $\hat{p}$ with $\hat{p}_{abc} = p_{(1-a)bc}$, $a, b, c \in \{0, 1\}$. This has the following implications to the covariances.

$$
\tau_{\alpha\beta} = p_{11\Sigma} - p_{1\Sigma \Sigma} p_{\Sigma 1\Sigma} = (p_{\Sigma 1\Sigma} - p_{01\Sigma}) - p_{1\Sigma \Sigma} p_{\Sigma 1\Sigma}
$$

$$
= -p_{01\Sigma} + p_{\Sigma 1\Sigma} (1 - p_{1\Sigma \Sigma}) = -(p_{01\Sigma} - p_{0\Sigma \Sigma} p_{\Sigma 1\Sigma})
$$

$$
= -(p_{1\Sigma \Sigma} - \hat{p}_{1\Sigma \Sigma} \hat{p}_{\Sigma 1\Sigma}) = -\hat{\tau}_{\alpha\beta}.
$$

and analogously $\hat{\tau}_{\alpha\gamma} = -\tau_{\alpha\gamma}$ and $\hat{\tau}_{\beta\gamma} = \tau_{\beta\gamma}$. Thus, if $\tau_{\alpha\beta}$ and $\tau_{\alpha\gamma}$ are smaller than zero, then a state flip produces positive covariances and the sign for the overall product remains the same.

Proof of Lemma 2. Using the Markov invariants from Section 6 we immediately see, that if $\tau_{\alpha\beta} = 0$ due to $M_{11}^\alpha - M_{11}^\alpha = 0$ then also $\tau_{\alpha\gamma} = 0$ and $\tau_{\alpha\beta\gamma} = 0$. If $q_{1\zeta}^\gamma \in \{0, 1\}$ then all four covariances are zero.

For point 2 regard (19). But this term will be non-negative as long as $q_{1\zeta}^\gamma$ is a probability, which is a model condition. This completes the proof.

Proof of Corollary 3. Select one leaf $\alpha \in L$ and define $L_0 = \{\beta : \tau_{\alpha\beta} < 0\}$. Flipping the states in $L_0$ gives us $\tau_{\alpha\beta} > 0$ for all $\beta \in L, \beta \neq \alpha$ by Lemma 1. Fix now $\beta \neq \beta' \in L \setminus \{\alpha\}$. Then $\alpha, \beta, \beta'$, together with the root $\zeta$ of the tree, define uniquely a tripod tree and the restriction of $p$ to $\alpha, \beta, \beta'$ must obey the tripod equations. Using Lemma 2(2), on this tripod tree shows now that $\tau_{\alpha\beta} \tau_{\alpha\beta'} \tau_{\beta\beta'} > 0$. This implies that $\tau_{\beta\beta'}$ is positive, too.

Proof of Corollary 4. A triplet distribution $p$ for which only one covariance is zero does not satisfy Lemma 2(1) and hence is not tripod decomposable. Further, by looking at (16) we see that there is also no real- or complex-valued parameter set that would yield only one zero covariance. Hence, such a triplet distribution would also not be algebraically decomposable.
Proof of Lemma 3. We insert the refined parameters into the tripod equations to get:

\[ p_{abc} = q_1^c M_{1a}^\alpha M_{1b}^\beta M_{1c}^\gamma + (1 - q_1^c) M_{0a}^\alpha M_{0b}^\beta M_{0c}^\gamma, \]

i.e. the tripod equations are recovered with flipped parameters. This completes the proof.

Proof of Theorem 5. We derive the parameters from the tripod equations. As mentioned in Section 3.1 there is a linear relationship between \( p \) and its marginalisations. Thus, finding a solution for the tripod equations is equivalent to finding the solution for the following set of equations

\[
\begin{align*}
\varepsilon_{\alpha\beta\gamma} &= q_1^c M_{11}^\alpha M_{11}^\beta M_{11}^\gamma + (1 - q_1^c) M_{01}^\alpha M_{01}^\beta M_{01}^\gamma, \quad (A.1) \\
\varepsilon_{\alpha\beta} &= q_1^c M_{11}^\alpha M_{11}^\beta + (1 - q_1^c) M_{01}^\alpha M_{01}^\beta, \quad (A.2) \\
\varepsilon_{\alpha\gamma} &= q_1^c M_{11}^\alpha M_{11}^\gamma + (1 - q_1^c) M_{01}^\alpha M_{01}^\gamma, \quad (A.3) \\
\varepsilon_{\beta\gamma} &= q_1^c M_{11}^\beta M_{11}^\gamma + (1 - q_1^c) M_{01}^\beta M_{01}^\gamma, \quad (A.4) \\
\varepsilon_{\alpha} &= q_1^c M_{11}^\gamma + (1 - q_1^c) M_{01}^\gamma, \quad (A.5) \\
\varepsilon_{\beta} &= q_1^c M_{11}^\beta + (1 - q_1^c) M_{01}^\beta, \quad (A.6) \\
\varepsilon_{\gamma} &= q_1^c M_{11}^\gamma + (1 - q_1^c) M_{01}^\gamma. \quad (A.7)
\end{align*}
\]

Equations (A.5)-(A.7) yield

\[ (1 - q_1^c) M_{01}^\alpha = \varepsilon_{\alpha} - q_1^c M_{11}^\alpha, \quad (1 - q_1^c) M_{01}^\beta = \varepsilon_{\beta} - q_1^c M_{11}^\beta, \quad (1 - q_1^c) M_{01}^\gamma = \varepsilon_{\gamma} - q_1^c M_{11}^\gamma. \quad (A.8) \]

Inserting (A.8) into (A.2) returns

\[
\begin{align*}
(1 - q_1^c) \varepsilon_{\alpha\beta} &= q_1^c (1 - q_1^c) M_{11}^\alpha M_{11}^\beta + (\varepsilon_{\alpha} - q_1^c M_{11}^\alpha)(\varepsilon_{\beta} - q_1^c M_{11}^\beta) \\
&= q_1^c M_{11}^\alpha M_{11}^\beta + \varepsilon_{\alpha} \varepsilon_{\beta} - q_1^c (\varepsilon_{\alpha} M_{11}^\beta + \varepsilon_{\beta} M_{11}^\alpha),
\end{align*}
\]

and in consequence

\[
\begin{align*}
q_1^c M_{11}^\beta (M_{11}^\alpha - \varepsilon_{\alpha}) &= \tau_{\alpha\beta} + q_1^c (\varepsilon_{\beta} M_{11}^\alpha - \varepsilon_{\alpha\beta}), \quad (A.9) \\
q_1^c M_{11}^\alpha (M_{11}^\gamma - \varepsilon_{\alpha}) &= \tau_{\alpha\gamma} + q_1^c (\varepsilon_{\gamma} M_{11}^\gamma - \varepsilon_{\alpha\gamma}). \quad (A.10)
\end{align*}
\]

We insert (A.9), (A.10) back into (A.8)

\[
\begin{align*}
(1 - q_1^c) M_{01}^\beta (M_{01}^\alpha - \varepsilon_{\alpha}) &= \varepsilon_{\beta} (M_{11}^\alpha - \varepsilon_{\alpha}) - \tau_{\alpha\beta} - q_1^c (\varepsilon_{\beta} M_{11}^\alpha - \varepsilon_{\alpha\beta}) \\
&= (1 - q_1^c)(\varepsilon_{\beta} M_{11}^\alpha - \varepsilon_{\alpha\beta}).
\end{align*}
\]
In the case of $q_1^\zeta = 1$ we get from (A.5) and (A.2) that $M_{11}^\alpha = \varepsilon_\alpha$ and $\varepsilon_{\alpha\beta} = \varepsilon_\alpha\varepsilon_\beta$. Hence, we remove $1 - q_1^\zeta$ from the above equation without destroying equality. Thus, we get

$$M_{01}^\beta(M_{11}^\alpha - \varepsilon_\alpha) = \varepsilon_\beta M_{11}^\alpha - \varepsilon_{\alpha\beta}, \quad (A.11)$$

$$M_{01}^\gamma(M_{11}^\alpha - \varepsilon_\alpha) = \varepsilon_\gamma M_{11}^\alpha - \varepsilon_{\alpha\gamma}. \quad (A.12)$$

We insert (A.8) in (A.1) to get

$$M_{11}^\alpha\varepsilon_\beta\gamma - \varepsilon_{\alpha\beta\gamma} = M_{01}^\beta M_{01}^\gamma(M_{11}^\alpha - \varepsilon_\alpha).$$

Applying (A.11) and (A.12) to this gives us

$$0 = (M_{11}^\alpha\varepsilon_\beta\gamma - \varepsilon_{\alpha\beta\gamma})(M_{11}^\alpha - \varepsilon_\alpha) - (\varepsilon_\beta M_{11}^\alpha - \varepsilon_{\alpha\beta})(\varepsilon_\gamma M_{11}^\alpha - \varepsilon_{\alpha\gamma})$$

$$= (M_{11}^\alpha)^2 \tau_{\beta\gamma} - M_{11}^\alpha(\tau_{\alpha\beta\gamma} + 2\varepsilon_\alpha \tau_{\beta\gamma}) + \varepsilon_{\alpha\beta\gamma}\varepsilon_\alpha - \varepsilon_{\alpha\beta}\varepsilon_{\alpha\gamma}.$$

We can apply the solution formula for quadratic equations provided $\tau_{\beta\gamma} \neq 0$, i.e. our condition (5) is satisfied. In that case we get

$$(M_{11}^\alpha) = \frac{\tau_{\alpha\beta\gamma} + 2\varepsilon_\alpha \tau_{\beta\gamma}}{2\tau_{\beta\gamma}} \pm \sqrt{\frac{(\tau_{\alpha\beta\gamma} + 2\varepsilon_\alpha \tau_{\beta\gamma})^2 - 4(\varepsilon_\alpha\varepsilon_\alpha - \varepsilon_{\alpha\beta}\varepsilon_{\alpha\gamma})\tau_{\beta\gamma}}{2\tau_{\beta\gamma}}}$$

$$= \varepsilon_\alpha + \frac{\tau_{\alpha\beta\gamma} \pm \sqrt{\tau_{\alpha\beta\gamma}^2 + 4\varepsilon_\alpha\varepsilon_\alpha\tau_{\beta\gamma}}}{2\tau_{\beta\gamma}}. \quad (A.13)$$

Thus we have established the term for $M_{11}^\alpha$. The next step is to derive $q_1^\zeta$. We insert (A.9)- (A.12) into (A.4) and get

$$q_1^\zeta(M_{11}^\alpha - \varepsilon_\alpha)^2 \varepsilon_{\beta\gamma} = (\tau_{\alpha\beta} + q_1^\zeta(\varepsilon_\beta M_{11}^\alpha - \varepsilon_{\alpha\beta}))(\tau_{\alpha\gamma} + q_1^\zeta(\varepsilon_\gamma M_{11}^\alpha - \varepsilon_{\alpha\gamma}))$$

$$+ q_1^\zeta(1 - q_1^\zeta)(\varepsilon_\beta M_{11}^\alpha - \varepsilon_{\alpha\beta})(\varepsilon_\gamma M_{11}^\alpha - \varepsilon_{\alpha\gamma})$$

$$= (1 - q_1^\zeta)\tau_{\alpha\beta}\tau_{\alpha\gamma} + q_1^\zeta\varepsilon_{\beta\gamma}(M_{11}^\alpha - \varepsilon_\alpha)^2$$

and hence we get the quadratic relation

$$0 = (1 - q_1^\zeta)\tau_{\alpha\beta}\tau_{\alpha\gamma} - q_1^\zeta\tau_{\beta\gamma}(M_{11}^\alpha - \varepsilon_\alpha)^2 \quad (A.14)$$

We insert (A.13) and get

$$\tau_{\alpha\beta}\tau_{\alpha\gamma} = q_1^\zeta(\tau_{\alpha\beta}\tau_{\alpha\gamma} + \tau_{\beta\gamma}(M_{11}^\alpha - \varepsilon_\alpha)^2),$$

$$4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} = q_1^\zeta(4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} + (\tau_{\alpha\beta\gamma} + \sqrt{\chi})^2),$$

$$4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} = 2q_1^\zeta\sqrt{\chi}(\sqrt{\chi} + \tau_{\alpha\beta\gamma}).$$

We use the equality

$$4\tau_{\alpha\beta}\tau_{\alpha\gamma}\tau_{\beta\gamma} = \chi - \tau_{\alpha\beta\gamma}^2 = (\sqrt{\chi} + \tau_{\alpha\beta\gamma})(\sqrt{\chi} - \tau_{\alpha\beta\gamma}).$$
and the observation that \( \sqrt{\chi} (\sqrt{\chi} - \tau_{\alpha\beta\gamma}) = 0 \) if and only if the conditions in (5) are violated to get

\[
q_1^C = \frac{\sqrt{\chi} - \tau_{\alpha\beta\gamma}}{2\sqrt{\chi}} = \frac{1}{2} - \frac{\tau_{\alpha\beta\gamma}}{2\sqrt{\chi}}, \tag{A.15}
\]

thus inferring the proposed term for \( q_1^C \). Next we infer the term for \( M_{01}^\alpha \). To this end we insert (A.13) and (A.15) into (A.8):

\[
- q_1^C (M_{11}^\alpha - \varepsilon_\alpha) = (1 - q_1^C) (M_{01}^\alpha - \varepsilon_\alpha),
\]

\[
(\tau_{\alpha\beta\gamma} - \sqrt{\chi}) (\tau_{\alpha\beta\gamma} + \sqrt{\chi}) = 2\tau_{\beta\gamma} (\tau_{\alpha\beta\gamma} + \sqrt{\chi}) (M_{01}^\alpha - \varepsilon_\alpha),
\]

\[
M_{01}^\alpha = \varepsilon_\alpha + \frac{\tau_{\alpha\beta\gamma} - \sqrt{\chi}}{2\tau_{\beta\gamma}},
\]

thus inferring the proposed term. The remaining terms are inferred analogously. This completes the proof. \( \square \)

**Proof of Theorem 7**. We bound the parameters from (6) between 0 and 1:

\[
0 \leq \frac{1}{2} - \frac{\tau_{\alpha\beta\gamma}}{2\sqrt{\chi}} \leq 1,
\]

\[- \sqrt{\chi} \leq \tau_{\alpha\beta\gamma} \leq \sqrt{\chi},
\]

\[
0 \leq \tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma}.
\]

With (5) this yields positivity for the unconditional covariances. Next we look at \( M_{01}^\alpha \) and \( M_{11}^\alpha \):

\[
0 \leq \varepsilon_\alpha + \frac{\tau_{\alpha\beta\gamma} - \sqrt{\chi}}{2\tau_{\beta\gamma}} \leq 1,
\]

\[- 2\varepsilon_\alpha \tau_{\beta\gamma} \leq \tau_{\alpha\beta\gamma} - \sqrt{\chi} \leq 2(1 - \varepsilon_\alpha) \tau_{\beta\gamma},
\]

\[
\tau_{\alpha\beta\gamma} - 2(1 - \varepsilon_\alpha) \tau_{\beta\gamma} \leq \sqrt{\chi} \leq \tau_{\alpha\beta\gamma} + 2\varepsilon_\alpha \tau_{\beta\gamma}
\]

and

\[
0 \leq \varepsilon_\alpha + \frac{\tau_{\alpha\beta\gamma} + \sqrt{\chi}}{2\tau_{\beta\gamma}} \leq 1,
\]

\[- 2\varepsilon_\alpha \tau_{\beta\gamma} \leq \tau_{\alpha\beta\gamma} + \sqrt{\chi} \leq 2(1 - \varepsilon_\alpha) \tau_{\beta\gamma},
\]

\[- (2\varepsilon_\alpha \tau_{\beta\gamma} + \tau_{\alpha\beta\gamma}) \leq \sqrt{\chi} \leq 2(1 - \varepsilon_\alpha) \tau_{\beta\gamma} - \tau_{\alpha\beta\gamma}.
\]

Squaring both inequalities reduces the four inequalities to the following two:

\[
\tau_{\alpha\beta\gamma}^2 + 4\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \leq (2\varepsilon_\alpha \tau_{\beta\gamma} + \tau_{\alpha\beta\gamma})^2, \tag{A.16}
\]

\[
\tau_{\alpha\beta\gamma}^2 + 4\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \leq (2(1 - \varepsilon_\alpha) \tau_{\beta\gamma} - \tau_{\alpha\beta\gamma})^2. \tag{A.17}
\]
We look first at inequality (A.16) and get
\[
\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \leq \varepsilon_{\alpha} \tau_{\beta\gamma}^2 + \varepsilon_{\alpha} \tau_{\beta\gamma} \tau_{\alpha\gamma},
\]
\[
0 \leq \varepsilon_{\alpha} (\varepsilon_{\alpha} \tau_{\beta\gamma} + \tau_{\alpha\gamma}) - \tau_{\alpha\beta} \tau_{\alpha\gamma},
\]
\[
0 \leq \varepsilon_{\alpha} \varepsilon_{\alpha\beta\gamma} - \varepsilon_{\alpha\beta} \varepsilon_{\alpha\gamma} = \tau_{\beta\gamma} | 1.\]

Set \( \hat{\varepsilon}_{\alpha} := (1 - \varepsilon_{\alpha}) = p_{001} \) and look at (A.17):
\[
\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \leq \hat{\varepsilon}_{\alpha} \tau_{\beta\gamma}^2 - \hat{\varepsilon}_{\alpha} \tau_{\alpha\beta} \tau_{\alpha\gamma},
\]
\[
0 \leq \hat{\varepsilon}_{\alpha} (\hat{\varepsilon}_{\alpha} \tau_{\beta\gamma} - \tau_{\alpha\beta} \tau_{\alpha\gamma}) - \tau_{\alpha\beta} \tau_{\alpha\gamma},
\]
\[
0 \leq p_{000} p_{011} - p_{001} p_{010} = \tau_{\beta\gamma} | 0.\]

Hence, we have derived the proposed inequalities. \( \square \)

Proof of Proposition 8. The tripod equations (4) imply:
\[
\chi = \tau_{\alpha\beta\gamma}^2 + 4\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} = (M_{11}^\alpha - M_{01}^\alpha)^2 (M_{11}^\beta - M_{01}^\beta)^2 (M_{11}^\gamma - M_{01}^\gamma)^2 (1 - q_1^\alpha)^2 (q_1^\alpha)^2
\]
Together with (18) and (16) we see that there is no set of real or complex parameters such that \( \chi = 0 \) but \( \tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma} \neq 0. \) \( \square \)

Proof of Proposition 9. The cases are easily verified by looking at Equation (16) and inserting the selected parameters back into (4). \( \square \)

Proof of Proposition 10. The function \( \chi : \mathbb{C}^8 \to \mathbb{C} \) is a nonconstant polynomial mapping. Thus the set \( \{ p \in \mathbb{R}^8 : \chi(p) = 0 \} \) is a Lebesgue zero set. The same holds for the set
\[
\{ p \in \mathbb{R}^8 : \tau_{\alpha\beta}(p) = 0 \text{ or } \tau_{\alpha\gamma}(p) = 0 \text{ or } \tau_{\beta\gamma}(p) = 0 \}.
\]
This completes the proof. \( \square \)

Proof of Proposition 11. We recover \( M^\psi \) by inserting the parameters from (6) into (11). To infer the invariants we first look at the equality conditions. We do this representatively by looking at \( M^\alpha = \tilde{M}^\alpha. \) In particular we look at
\[
\tilde{M}_{11}^\alpha - \tilde{M}_{01}^\alpha = \tilde{M}_{11}^\alpha - \tilde{M}_{01}^\alpha, \quad \tilde{M}_{11}^\alpha + \tilde{M}_{01}^\alpha = \tilde{M}_{11}^\alpha + \tilde{M}_{01}^\alpha,
\]
and thus
\[
\frac{\sqrt{\chi_{\alpha\beta\gamma}}}{\tau_{\beta\gamma}} = \frac{\sqrt{\chi_{\alpha\delta\gamma}}}{\tau_{\beta\delta}}, \quad \frac{\tau_{\alpha\beta\gamma}}{\tau_{\beta\gamma}} = \frac{\tau_{\alpha\gamma\delta}}{\tau_{\beta\delta}},
\]
\[
\frac{\tau_{\alpha\gamma}^2 + 4\tau_{\alpha\beta} \tau_{\alpha\gamma} \tau_{\beta\gamma}}{\tau_{\beta\gamma}^2} = \frac{\tau_{\alpha\delta}^2 + 4\tau_{\alpha\beta} \tau_{\alpha\delta} \tau_{\beta\delta}}{\tau_{\beta\delta}^2}, \quad \frac{\tau_{\alpha\beta\gamma}}{\tau_{\beta\gamma}} = \frac{\tau_{\alpha\gamma\delta}}{\tau_{\beta\delta}},
\]
\[
\frac{\tau_{\alpha\delta}}{\tau_{\beta\delta}} = \frac{\tau_{\alpha\gamma}}{\tau_{\beta\delta}}, \quad \frac{\tau_{\alpha\beta\gamma}}{\tau_{\beta\gamma}} = \frac{\tau_{\alpha\gamma}}{\tau_{\alpha\delta}}.
\]
Looking at $\mathbf{M}^\beta = \mathbf{\hat{M}}^\beta$ yields the same equalities. Reproducing the calculations for
$\mathbf{\hat{M}}^\gamma = \mathbf{M}^\gamma$ yields the invariants $f_1$ to $f_3$.

For the inference of $f_0$ observe that the equation system (2) can be written in a
marginalised form, i.e. one replaces the equations in $(p_{abcd})_{a,b,c,d \in \{0,1\}}$ by the linear
transforms $\varepsilon_{\alpha\beta\gamma\delta}$, $\varepsilon_{\alpha\beta\gamma}$, $\varepsilon_{\alpha\gamma\delta}$, $\varepsilon_{\beta\gamma\delta}$, $\varepsilon_{\alpha\beta}$, $\varepsilon_{\alpha\gamma}$, $\varepsilon_{\beta\gamma}$, $\varepsilon_{\beta\delta}$, $\varepsilon_{\gamma\delta}$, $\varepsilon_{\alpha}$, $\varepsilon_{\beta}$, $\varepsilon_{\gamma}$ and $\varepsilon_{\delta}$.

We immediately see that all terms but $\varepsilon_{\alpha\beta\gamma\delta}$ are covered by our investigation of
the tripod case. We insert the parameters obtained in (6) and (12) into the equation for
$\varepsilon_{\alpha\beta\gamma\delta}$ to get:

$$
\varepsilon_{\alpha\beta\gamma\delta} = (1 - q_1) \overline{M}_{01}^\alpha \overline{M}_{01}^\beta ((1 - M_{01}^\psi) \mathbf{\hat{M}}_{01}^\gamma \mathbf{\hat{M}}_{01}^\delta + M_{01}^\psi \mathbf{\hat{M}}_{11}^\gamma \mathbf{\hat{M}}_{11}^\delta)
+ q_1 \overline{M}_{11}^\alpha \overline{M}_{11}^\beta ((1 - M_{11}^\psi) \mathbf{\hat{M}}_{01}^\gamma \mathbf{\hat{M}}_{01}^\delta + M_{11}^\psi \mathbf{\hat{M}}_{11}^\gamma \mathbf{\hat{M}}_{11}^\delta).
$$

Reordering and restructuring this equation eventually yields invariant $f_0$. This
completes the proof. 

\textit{Proof of Proposition 12.} Theorem 7 covers the first part of the Proposition. The
remaining inequalities are obtained by bounding (12) between 0 and 1 and use the fact
that the covariances are always positive with Lemma 2(1):

$$
-1 \leq \frac{\tau_{\alpha\delta}\tau_{\alpha\beta\gamma} - \tau_{\alpha\beta}\tau_{\alpha\gamma\delta} - \tau_{\alpha\delta}\sqrt{X_{\alpha\beta\gamma}}}{\tau_{\alpha\beta}\sqrt{X_{\alpha\gamma\delta}}} \leq 1,
\varepsilon_{\alpha\beta}(\tau_{\alpha\gamma\delta} - \sqrt{X_{\alpha\gamma\delta}}) \leq \tau_{\alpha\delta}(\tau_{\alpha\beta\gamma} - \sqrt{X_{\alpha\beta\gamma}}) \leq \tau_{\alpha\beta}(\tau_{\alpha\gamma\delta} + \sqrt{X_{\alpha\gamma\delta}}),
-1 \leq \frac{\tau_{\alpha\delta}\tau_{\alpha\beta\gamma} - \tau_{\alpha\beta}\tau_{\alpha\gamma\delta} + \tau_{\alpha\delta}\sqrt{X_{\alpha\beta\gamma}}}{\tau_{\alpha\beta}\sqrt{X_{\alpha\gamma\delta}}} \leq 1,
\varepsilon_{\alpha\beta}(\tau_{\alpha\gamma\delta} - \sqrt{X_{\alpha\gamma\delta}}) \leq \tau_{\alpha\delta}(\tau_{\alpha\beta\gamma} + \sqrt{X_{\alpha\beta\gamma}}) \leq \tau_{\alpha\beta}(\tau_{\alpha\gamma\delta} + \sqrt{X_{\alpha\gamma\delta}}),
$$

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| triplet | $M_0^{\alpha}$ | $M_{\beta}$ | $M_{\gamma}$ | $M_{\delta}$ | $q_\zeta$ |
|---------|----------------|-------------|-------------|-------------|---------|
| $\alpha\beta\gamma$ | 0.0417424 | 0.118119 | 0.172673 | 0 | 0.5 |
| $\alpha\beta\delta$ | 0.118119 | 0.0417424 | 0 | 0.172673 | 0.5 |
| $\alpha\gamma\delta$ | 0.172673 | 0 | 0.0417424 | 0.118119 | 0.5 |
| $\beta\gamma\delta$ | 0 | 0.172673 | 0.118119 | 0.0417424 | 0.5 |

Table A.1: The parameters for each triplet.