A SEMIALGEBRAIC DESCRIPTION OF THE GENERAL MARKOV MODEL ON PHYLOGENETIC TREES

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Abstract. Many of the stochastic models used in inference of phylogenetic trees from biological sequence data have polynomial parameterization maps. The image of such a map — the collection of joint distributions for a model — forms the model space. Since the parameterization is polynomial, the Zariski closure of the model space is an algebraic variety which is typically much larger than the model space, but has been usefully studied with algebraic methods. Of ultimate interest, however, is not the full variety, but only the model space. Here we develop complete semialgebraic descriptions of the model space arising from the k-state general Markov model on a tree, with slightly restricted parameters. Our approach depends upon both recently-formulated analogs of Cayley's hyperdeterminant, and the construction of certain quadratic forms from the joint distribution whose positive (semi-)definiteness encodes information about parameter values. We additionally investigate the use of Sturm sequences for obtaining similar results.

Key words. phylogenetic tree, phylogenetic variety, semialgebraic set, general Markov model

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1. Introduction. Statistical inference of evolutionary relationships among organisms from DNA sequence data is routinely performed using probabilistic models of sequence evolution along a tree. A site in a sequence is viewed as a 4-state (A,C,G, T) random variable, which undergoes state changes as it descends along the tree from an ancestral organism to its modern descendants. Such models exhibit a rich mathematical structure, which reflects both the combinatorial features of the tree, and the algebraic way in which stochastic matrices associated to edges of the tree are combined to produce a joint probability distribution describing sequences of the extant organisms.

One thread in the extensive literature on such models has utilized the viewpoint of algebraic geometry to understand the probability distributions that may arise. This is natural, since the distributions are in the image of a polynomial map, and the image thus lies in an algebraic variety. The defining equations of this variety (which depend on the tree topology), are called *phylogenetic invariants*. That a probability distribution satisfies them can be taken as evidence that it arose from sequence evolution along the particular tree. Phylogenetic invariants and varieties have been extensively studied by many authors [13, 26, 17, 21, 20, 3, 34, 8, 12, 30, 11] (see [7] for more references) with goals ranging from biological (improving data analysis) to statistical (establishing the identifiability of model parameters) to purely mathematical.

However, it has long been understood that, in addition to the equalities of phylogenetic invariants, inequalities should play a role in characterizing those distributions actually of interest for statistical purposes. Much of a phylogenetic variety is typically composed of points not arising from stochastic parameters, but rather from applying the same polynomial parameterization map to complex parameters. Thus the model space — the set of probability distributions arising as the image of stochastic parameters on a tree — can be considerably smaller than the set of all probability

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distributions on the variety. An instructive recent computation [37] demonstrated that for the 2-state general Markov model on the 3-leaf tree, for example, the model space is only about 8% of the nonnegative real points on the variety. Inequalities can thus be crucial in determining if a probability distribution arises from a model.

In the pioneering 1987 paper of Cavender and Felsenstein [13] polynomial equalities and inequalities are given that can test which of the 3 possible unrooted leaf-labeled 4-leaf trees might have produced a given probability distribution, and thus in principle determine evolutionary relationships between 4 organisms. Nonetheless, despite many advances in understanding phylogenetic invariants in the intervening years, little has been accomplished in finding or understanding the necessary inequalities. The potential usefulness of such inequalities, meanwhile, has been demonstrated in [18], where an inequality that holds for the 2-state model on all tree topologies plays a key role in studying loss of biodiversity under species extinction. In [9] a small number of inequalities, dependent on the tree, were used to show that for certain mixture models trees were identifiable from probability distributions.

Recent independent works by Smith and Zwiernik [37] and by Klaere and Liebscher [23] provided the first substantial progress on the general problem of finding sufficient inequalities to describe the model space. Both groups successfully formulated inequalities for the 2-state general Markov model on trees, using different viewpoints. While the 2-state model has some applicability to DNA sequences, through a purine/pyrimidine encoding of nucleotides, it is unfortunately not clear how to extend these works to the more general k-state model, or even to the particular $k = 4$ model that is directly applicable to DNA. Features of the statistical framework in [37] make generalizing to more states highly problematic, while the formulation of [23] involves beating through a thicket of algebraic details which are similarly difficult to generalize.

In this work we provide a third approach to understanding the model space of the general Markov model on trees which has the advantage of extending from the 2-state to the k-state model with little modification. Our goal is a semialgebraic description (given by a boolean combination of polynomial equalities and inequalities) of the set of probability distributions that arise on a specific tree. Such a description exists by the Tarski-Seidenberg Theorem [36, 31], since the stochastic parameter space for any k-state general Markov model is a semialgebraic set, so its image under the polynomial parameterization map must be as well. However, we seek an explicit description, and this theorem does not provide a useful means of obtaining it.

We describe below two methods for obtaining such a semialgebraic model description. In one approach, that applies equally easily to all k and all binary trees, we obtain inequalities using a recently-formulated analog of Cayley's $2 \times 2 \times 2$ hyperdeterminant from [1], and the construction of certain quadratic forms from the joint distribution whose positive (semi-)definiteness encodes information about parameter values. We note that the appearance of the hyperdeterminant in both [37] and [23] motivated the work of [1], but that our introduction of quadratic forms in this paper is an equally essential tool for obtaining our results. Moreover, we do not see direct precursors of this idea in either [37] or [23].

We also describe an alternative method using Sturm sequences for univariate polynomials to obtain inequalities. Specifically, we construct polynomials in the entries of a probability distribution whose roots are exactly a subset of the numerical parameters, and Sturm theory leads to inequalities stating that the roots lie in the interval $(0, 1)$, as the parameters must. Although for the 2-state model this leads to a complete semialgebraic description of the model on a 3-leaf tree, for higher k it becomes more unwieldy. Nonetheless, this approach can produce inequalities of smaller degree than those found using quadratic forms, so we consider it a potentially useful technique.

In both approaches, we must impose some restrictions on the set of stochastic parameters in order to give our semialgebraic conditions. We thus formulate a notion of *nonsingular parameters* and mostly restrict to considering them for our results. In the $k = 2$ case this notion is particularly natural from a statistical point of view, though it is slightly less so for higher k. Indeed, an understanding of why this notion is needed algebraically illuminates, we believe, the difficulties of passing from 2-state results to k-state results.

This paper is organized as follows: In §2 we formally introduce the general Markov model on trees and set basic notations and terminology, including the notion of nonsingular parameters. In §3, we give a semialgebraic description of the general Markov model on the 3-leaf tree using the work of [1] and Sylvester's theorem on quadratic forms, a description that is made complete for the 2-state model, but holds only for nonsingular parameters of the k-state model. Additionally, we discuss connections to several previous works on the 2-state model [29, 37, 23]. In §4, we use Sturm sequences to give partial semialgebraic descriptions of 3-leaf model spaces, and develop several examples. In §5, we give the main result: a semialgebraic description of the k-state general Markov model on n-leaf trees for nonsingular parameters. For the 2-state model we prove a slightly stronger result that drops the nonsingularity assumption.

2. Definitions and Notations.

2.1. The general Markov model on trees. We review the k-state general Markov model on trees, GM(k), whose parameters consist of a combinatorial object, a tree, and a collection of numerical parameters that are associated to a rooted version of the tree.

Let $T = (V, E)$ be a binary tree with leaves $L \subseteq V$, $|L| = n$, and $\{X_a\}_{a \in V}$ a collection of discrete random variables associated to the nodes, all with state space $[k] = \{1, 2, \ldots, k\}$. Distinguish an internal node r of T to serve as its root, and direct all edges of T away from r. (Often this model is presented with the root as a node of valence 2 which is introduced by subdividing some edge. However, under very mild assumptions this leads to the same probability distributions we consider here [33, 3], so we avoid that complication.) Though necessary for parameterizing the model, the choice of r will not matter in our final results, as will be shown in §5.

For a tree T rooted at r, numerical parameters $\{\boldsymbol{\pi}, \{M_e\}_{e\in E}\}$ for the GM(k) model on T are:

(i) A *root distribution* row vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k)$, with nonnegative entries summing to 1;

(ii) *Markov matrices* M_e, with nonnegative entries and row sums equal to 1.

The vector $\boldsymbol{\pi}$ specifies the distribution of the random variable X_r, *i.e.*, $\pi_i = \mathrm{Prob}(X_r = i)$, and the Markov matrices M_e, for $e = (a_e, b_e) \in E$, give transition probabilities $M_e(i, j) = \mathrm{Prob}(X_{b_e} = j \mid X_{a_e} = i)$ of the various state changes in passing from the parent vertex a_e to the child vertex b_e. Letting $\mathbf{X} = (X_a)_{a\in V}$, the joint probability distribution at all nodes of T is thus

$$\mathrm{Prob}(\mathbf{X} = \mathbf{j}) = \pi_{j_r} \prod_{e\in E} M_e(j_{a_e}, j_{b_e}).$$

By marginalizing over all variables at internal nodes of T, we obtain the *joint distribution, P, of states at the leaves of T*; if $\mathbf{k} \in [k]^{|L|}$ is an assignment of states to leaf variables, then

$$P(\mathbf{k}) = \sum_{\mathbf{m} \in [k]^{|V \smallsetminus L|}} \operatorname{Prob}(\mathbf{X} = (\mathbf{k}, \mathbf{m}))$$

where $(\mathbf{k}, \mathbf{m})$ is an assignment of states to all the vertices of T compatible with $\mathbf{k}$. It is natural to view P as an n-dimensional $k \times \cdots \times k$ array, or *tensor*, with one index for each leaf of the tree.

For fixed T and choice of r, we use ψ_T to denote the *parameterization map*

$$\psi_T : \{\boldsymbol{\pi}, \{M_e\}_{e \in E}\} \mapsto P.$$

That the coordinate functions of ψ_T are polynomial is obvious, but essential to our work here. Note that we may naturally extend the domain of the polynomial map to larger sets, by dropping the nonnegativity assumptions in (i) and (ii), but retaining the condition that rows must sum to 1. We will consider *real parameters* and a real parameterization map, as well as *complex parameters* and a complex parameterization map. In contrast, we refer to the original probabilistic model as having *stochastic parameters*. Since the parameterization maps are all given by the same formula, we use ψ_T to denote them all, but will always indicate the current domain of interest.

The image of complex, real, or stochastic parameters under ψ_T is an n-dimensional $k \times \cdots \times k$ tensor, whose k^n entries sum to 1. When parameters are not stochastic, this tensor generally does not specify a probability distribution, as there can be negative or complex entries. We refer to any tensor whose entries sum to 1, regardless of whether the entries are complex, real, or nonnegative, as a *distribution*, but reserve the term *probability distribution* for a nonnegative distribution. With this language, the image of complex parameters under ψ_T is a distribution, but may or may not be a probability distribution. Similarly, while the matrix parameters M_e have rows summing to one even for complex parameters, we reserve the term *Markov* matrix exclusively for the stochastic setting.

2.2. Algebraic and semialgebraic model descriptions. Most previous algebraic analysis of the GM(k) model has focused on the *algebraic variety* associated to it for each choice of tree T. With this viewpoint one is essentially passing from the parameterization of the model, as given above, to an implicit description of the image of the parameterization as a zero set of certain polynomial functions, traditionally called *phylogenetic invariants* [13, 26, 7].

Whether one considers stochastic, real, or complex parameters, the collection of phylogenetic invariants for GM(k) on a tree T are the same. Thus they cannot distinguish probability distributions that arise from stochastic parameters from those arising from non-stochastic real or complex ones. To complicate matters further, there exist distributions that satisfy all phylogenetic invariants for the model on a given tree, but are not even in the image of complex parameters. Though the algebraic issues behind this are well understood, they prevent classical algebraic geometry from being a sufficient tool to focus exclusively on the distributions of statistical interest.

To gain a more detailed understanding, we seek to refine the algebraic description of the model given by phylogenetic invariants into a *semialgebraic* description: In addition to finding polynomials vanishing on the image of the parameterization (or equivalently polynomial equalities holding at all points on the image), we also seek polynomial inequalities sufficient to distinguish the stochastic image precisely.

Recall that a subset of $\mathbb{R}^n$ is called a *semialgebraic set* if it is a boolean combination of sets each of which is defined by a single polynomial equality or inequality. The Tarski-Seidenberg Theorem [36, 31] implies that the image of a semialgebraic set under a polynomial map is also semialgebraic.

Since for all T the stochastic parameter space of ψ_T is clearly semialgebraic, this implies that semialgebraic descriptions exist for the images of the ψ_T. Determining such descriptions explicitly is our goal.

2.3. Nonsingular parameters, positivity, and independence. Some of our results will be stated with additional mild conditions placed on the allowed parameters for the GM(k) model. We state these conditions here, and explore their meaning.

DEFINITION 2.1. *A choice* $\{\boldsymbol{\pi}, \{M_e\}_{e\in E}\}$ *of stochastic, real, or complex parameters for* GM(k) *on a tree T with root r is said to be* nonsingular *provided*

(i) *at every (hidden or observed) node a, the marginal distribution $\mathbf{v}_a$ of X_a has no zero entry, and*

(ii) *for every edge e, the matrix M_e is nonsingular.*

Parameters which are not nonsingular are said to be singular*.*

For stochastic parameters, the first condition in this definition can be replaced with a simpler one:

(i') *the root distribution $\boldsymbol{\pi}$ has no zero entry.*

Statement (i) follows from (i') and (ii) inductively, since if all entries of $\mathbf{v}_a$ are positive and $M_{(a,b)}$ is a nonsingular Markov matrix, then the distribution $\mathbf{v}_b = \mathbf{v}_a M_{(a,b)}$ at a child b of a has positive entries. However, for complex or real parameters requirement (i) is not implied by (i') and (ii), as a simple example shows: $\mathbf{v}_a = (1/2, 1/2)$, and $M_{(a,b)} = \begin{pmatrix} s & 1-s \\ 2-s & s-1 \end{pmatrix}$ are singular parameters since $\mathbf{v}_b = (1, 0)$, even though $\mathbf{v}_a$ has no zero entries and $M_{(a,b)}$ is a nonsingular for $s \neq 1$.

It is also natural to require that all numerical parameters of GM(k) on a tree T be strictly positive. This means that all states may occur at the root, and every state change is possible in passing along any edge of the tree. This assumption is plausible from a modeling point of view, and can be desirable for technical statistical issues as well. Note that positivity of parameters does not ensure nonsingularity, since a Markov matrix may be singular despite all its entries being greater than zero. Similarly, nonsingularity of parameters does not ensure positivity since a nonsingular Markov matrix may have zero entries.

Given a joint probability distribution of random variables, two subsets of variables are *independent* when the marginal distribution for the union of the sets is the product of the marginal distributions for the two sets individually. We also use this term, in a nonstandard way, to apply to complex or real distributions when the same factorization holds.

To illustrate this usage, consider a tree T with two nodes, r, a and one edge (r, a). For complex parameters $\boldsymbol{\pi}$ and $M_{(r,a)}$, the joint distribution of X_r and X_a is given by the matrix

$$P = \operatorname{diag}(\boldsymbol{\pi}) M_{(r,a)}.$$

Then the variables are independent exactly when P is a rank 1 matrix: $P = \boldsymbol{\pi}^T \mathbf{v}_a$. For $k = 2$ this occurs precisely when the parameters are singular. For $k > 2$, however, independence implies the parameters are singular, but not *vice versa*. In general, singular parameters ensure that P has rank strictly less than k, but not that P has rank 1.

These comments easily extend to larger trees to give the following.

Proposition 2.2. *Suppose $P = \psi_T(\boldsymbol{\pi}, \{M_e\})$ for a choice of complex GM(k) parameters on an n-leaf tree T. If the parameters are nonsingular, then there is no proper partition of the indices of P into independent sets. For $k = 2$, the converse also holds.*

That the converse is false for $k > 2$ is a complicating factor for the generalization of our results from the $k = 2$ case. Indeed, this is the reason we ultimately restrict to nonsingular parameters.

In closing this section, we note that for any $P \in \mathrm{Im}(\psi_T)$, there is an inherent and well-understood source of non-uniqueness of parameters giving rise to P, sometimes called 'label-swapping.' Since internal nodes of T are unobservable variables, the distribution P is computed by summing over all assignments of states to such variables. As a result, if the state names were permuted for such a variable, and corresponding changes made in numerical parameters, P is left unchanged. Thus parameters leading to P can be determined at most up to such permutations.

In the case of nonsingular parameters, label-swapping is the only source of non-uniqueness of parameters leading to P [15]. (See also [25, 2]). For singular parameters there are additional sources of non-uniqueness.

2.4. Marginalizations, slices, group actions, and flattenings. Viewing probability distributions on n variables as n-dimensional tensors gives natural associations between statistical notions and tensor operations. For example, summing tensor entries over an index, or a collection of indices, corresponds to marginalizing over a variable, or collection of variables. Considering only those entries with a fixed value of an index, or collection of indices, corresponds (after renormalization) to conditioning on an observed variable, or collection of variables. Rearranging array entries into a new array, with fewer dimensions but larger size, corresponds to agglomerating several variables into a composite one with larger state space. Here we introduce the necessary notation to formalize these tensor operations.

Definition 2.3. *For an n-dimensional $k \times \cdots \times k$ tensor P, integer $i \in [n]$, and vector $\mathbf{v} = (v_1, \cdots, v_k)$, define the $(n-1)$-dimensional tensor $P *_i \mathbf{v}$ by*

$$(P *_i \mathbf{v})(j_1, \ldots, \hat{j}_i, \ldots, j_n) = \sum_{j_i=1}^{k} v_{j_i} P(j_1, \cdots, j_i, \cdots, j_n),$$

where $\hat{}$ denotes omission.

Thus, the ℓth slice of P in the ith index *is defined by $P_{\cdots\ell\cdots} = P *_i \mathbf{e}_\ell$, where $\mathbf{e}_\ell$ is the ℓth standard basis vector, and the ith* marginalization of P *is $P_{\cdots+\cdots} = P *_i \mathbf{1}$ where $\mathbf{1}$ is the vector of all 1s.*

The above product of a tensor and vector extends naturally to tensors and matrices.

Definition 2.4. *For an n-dimensional $k \times \cdots \times k$ tensor P and $k \times k$ matrix M, define the n-dimensional tensor $P *_i M$ by*

$$(P *_i M)(j_1, \ldots, j_n) = \sum_{\ell=1}^{k} P(j_1, \ldots, j_{i-1}, \ell, j_{i+1}, \ldots, j_n) M(\ell, j_i).$$

If the above operations on a tensor by vectors or matrices are performed in different indices, then they commute. This allows the use of n-tuple notation for the operation of matrices in all indices of a tensor, such as the following:

$$P \cdot (M_1, M_2, \ldots, M_n) = (\cdots((P *_1 M_1) *_2 M_2)\cdots) *_n M_n.$$

Although the M_i need not be invertible, restricting to that case gives the natural (right) group action of $GL(k, \mathbb{C})^n$ on $k \times \cdots \times k$ tensors. This generalizes the familiar operation on 2-dimensional tensors P, *i.e.*, on matrices, where

$$P \cdot (M_1, M_2) = (P *_1 M_1) *_2 M_2 = M_1^T P M_2.$$

If $\mathbf{v} \in \mathbb{C}^k$, then $\mathrm{Diag}(\mathbf{v})$ denotes the 3-dimensional $k \times k \times k$ diagonal tensor whose only nonzero entries are the v_i in the (i, i, i) positions. That this notion is useful for the GM(k) model is made clear by the observation that for a 3-leaf star tree T, rooted at the central node,

$$\psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\}) = \mathrm{Diag}(\boldsymbol{\pi}) \cdot (M_1, M_2, M_3). \tag{2.1}$$

If P is an n-dimensional $k \times \cdots \times k$ tensor and $[n] = A \sqcup B$ is a disjoint union of nonempty sets, then the *flattening of P with respect to this bipartition*, $\mathrm{Flat}_{A|B}(P)$ is the $k^{|A|} \times k^{|B|}$ matrix with rows indexed by $\mathbf{i} \in [k]^{|A|}$ and columns indexed by $\mathbf{j} \in [k]^{|B|}$, with

$$\mathrm{Flat}_{A|B}(P)(\mathbf{i}, \mathbf{j}) = P(\mathbf{k}),$$

where $\mathbf{k} \in [k]^n$ has entries matching those of $\mathbf{i}$ and $\mathbf{j}$, appropriately ordered. Thus the entries of P are simply rearranged into a matrix, in a manner consistent with the original tensor structure. When P specifies a joint distribution for n random variables, this flattening corresponds to treating the variables in A and B as two agglomerate variables, with state spaces the product of the state spaces of the individual variables.

Notations such as $\mathrm{Flat}_{1|23}(P)$, for example, will be used to denote the matrix flattening obtained from a 3-dimensional tensor using the partition of indices $A = \{1\}$, $B = \{2, 3\}$. If e is an edge in an n-leaf tree, then e naturally induces a bipartition of the leaves, by removing the edge and grouping leaves according to the resulting connected components. A flattening for such a bipartition is denoted by $\mathrm{Flat}_e(P)$.

Finally, we note that flattenings naturally occur in the notion of independence: If $[n] = A \sqcup B$, then the sets are independent precisely when $\mathrm{Flat}_{A|B}(P)$ is a rank 1 matrix.

3. GM(k) on 3-leaf trees. In this section we derive a semialgebraic description of GM(k) on the 3-leaf tree, the smallest example of interest. Results for the 3-leaf tree also serve as a building block for the study of the model on larger trees in §5. For this section, then, T is fixed, with leaves 1, 2, 3 and root r at the central node.

When $k = 2$, Cayley's *hyperdeterminant* plays a critical role, as has already been highlighted in [38]. Though our formulation will be different, we take the hyperdeterminant as our starting point. For any $2 \times 2 \times 2$ tensor $A = (a_{ijk})$, the hyperdeterminant

$\Delta(A)$ [14, 19, 16] is

$$\Delta(A) = \big(a_{111}^2 a_{222}^2 + a_{112}^2 a_{221}^2 + a_{121}^2 a_{212}^2 + a_{122}^2 a_{211}^2\big) - 2\big(a_{111}a_{112}a_{221}a_{222} + a_{111}a_{121}a_{212}a_{222} + a_{111}a_{122}a_{211}a_{222} + a_{112}a_{121}a_{212}a_{221} + a_{112}a_{122}a_{221}a_{211} + a_{121}a_{122}a_{212}a_{211}\big) + 4\big(a_{111}a_{122}a_{212}a_{221} + a_{112}a_{121}a_{211}a_{222}\big).$$

The function Δ has the $GL(2,\mathbb{C})^3$-invariance property

$$\Delta(P \cdot (g_1, g_2, g_3)) = \det(g_1)^2 \det(g_2)^2 \det(g_3)^2 \Delta(P). \tag{3.1}$$

This fact, combined with a study of canonical forms for $GL(2,\mathbb{C})^3$-orbit representatives, leads to the following theorem.

Theorem 3.1 ([16], Theorem 7.1). *A complex $2 \times 2 \times 2$ tensor P is in the $\mathrm{GL}(2,\mathbb{C})^3$-orbit of $D = \mathrm{Diag}(1,1)$ if, and only if, $\Delta(P) \neq 0$. A real tensor is in the $\mathrm{GL}(2,\mathbb{R})^3$-orbit of D if, and only if, $\Delta(P) > 0$.*

Suppose that $k = 2$ and $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ arises from nonsingular parameters on T. Then, equation (2.1) states $P = \mathrm{Diag}(\boldsymbol{\pi}) \cdot (M_1, M_2, M_3)$, but letting $M_1' = \mathrm{diag}(\boldsymbol{\pi})M_1$ we also have

$$P = D \cdot (M_1', M_2, M_3).$$

Therefore $\Delta(P) > 0$ by the forward implication of Theorem 3.1. This hyperdeterminantal inequality can thus be included in building a semialgebraic description of the GM(2) model when restricted to nonsingular parameters.

However, the inequality $\Delta(P) > 0$ yields a weaker conclusion than that P arises from stochastic, or even real, nonsingular parameters, so additional inequalities are needed for a semialgebraic model description.

Nonetheless, motivated by the role the hyperdeterminant plays in the semialgebraic description of the GM(2) model, in a separate work Allman, Jarvis, Rhodes, and Sumner [1] construct generalizations of Δ for $k \geq 2$. These functions are defined by

$$f_i(P; \mathbf{x}) = \det(H_{\mathbf{x}}(\det(P *_i \mathbf{x}))),$$

where $\mathbf{x}$ is a vector of auxiliary variables, and $H_{\mathbf{x}}$ denotes the Hessian operator. They also have invariance properties under $GL(k,\mathbb{C})^3$ such as

$$f_3(P \cdot (g_1, g_2, g_3); \mathbf{x}) = \det(g_1)^k \det(g_2)^k \det(g_3)^2 f_3(P; g_3\mathbf{x}).$$

The next theorem establishes that the nonvanishing of these polynomials, in conjunction with the vanishing of some others, identifies the orbit of $\mathrm{Diag}(\mathbf{1})$, and thus is an analog of Theorem 3.1 for larger k.

Theorem 3.2 ([1]). *A complex $k \times k \times k$ tensor P lies in the $GL(k,\mathbb{C})^3$-orbit of $\mathrm{Diag}(\mathbf{1})$ if, and only if, for some $i \in \{1,2,3\}$,*

(i) $(P *_i \mathbf{e}_j)\,\mathrm{adj}(P *_i \mathbf{x})(P *_i \mathbf{e}_\ell) - (P *_i \mathbf{e}_\ell)\,\mathrm{adj}(P *_i \mathbf{x})(P *_i \mathbf{e}_j) = 0$ *for all $j, \ell \in [k]$. Here* adj *denotes the classical adjoint, and equality means as a matrix of polynomials in* $\mathbf{x}$.

(ii) $f_i(P; \mathbf{x})$ *is not identically zero as a polynomial in* $\mathbf{x}$.

Moreover, if the enumerated conditions hold for one i, then they hold for all.

When $k > 2$ the $GL(k,\mathbb{C})^3$-orbit of $\mathrm{Diag}(\mathbf{1})$ is not dense among all $k \times k \times k$ tensors; rather its closure is a lower dimensional subvariety. This explains the necessity of the equalities in item (i). In the case $k = 2$ these equalities simplify to $0 = 0$ and thus hold for all tensors. One can further verify that if $k = 2$ then $f_i = \Delta$, so that Theorem 3.2 includes the first statement of Theorem 3.1.

One might hope that the polynomials $f_i(P; \mathbf{x})$ had a sign property similar to that given in Theorem 3.1 for $\Delta(P)$, so that a simple test could further distinguish the image of nonsingular real parameters. For $k = 3$, using functions related to the f_i, a semialgebraic description of the $GL(k,\mathbb{R})^3$-orbit of $\mathrm{Diag}(\mathbf{1})$ can in fact be obtained in this manner (see [1]), giving a complete analog of Theorem 3.1. However, for $k > 3$ no analog is known.

Finally, we emphasize that for $k > 2$ the functions f_i are *not* the ones usually referred to as hyperdeterminants [19], but rather a different generalization of Δ.

With semialgebraic conditions ensuring a tensor is in the $GL(k,\mathbb{C})^3$ orbit of $\mathrm{Diag}(\mathbf{1})$ in hand, we wish to supplement these to ensure it arises from nonsingular stochastic parameters. We address this in several steps; first, we give requirements that a tensor is the image of complex parameters under ψ_T, and then that these parameters be nonnegative.

Proposition 3.3. *Let P be a complex $k \times k \times k$ distribution. Then P is in the image of nonsingular complex parameters for GM(k) on the 3-leaf tree if, and only if, P is in the $GL(k,\mathbb{C})^3$-orbit of $\mathrm{Diag}(\mathbf{1})$ and $\det(P *_i \mathbf{1}) \neq 0$ for $i = 1, 2, 3$. Moreover, the parameters are unique up to label swapping.*

Proof. To establish the claimed reverse implication, suppose $P = \mathrm{Diag}(\mathbf{1}) \cdot (g_1, g_2, g_3)$ for some $g_i \in \mathrm{GL}(k,\mathbb{C})$, and let $\mathbf{r}^i = g_i\mathbf{1}$ denote the vector of row sums of g_i. A computation shows that

$$P *_3 \mathbf{1} = g_1^T \,\mathrm{diag}(\mathbf{r}^3) g_2.$$

Thus $\det(P *_3 \mathbf{1}) \neq 0$ is equivalent to the row sums of g_3 being nonzero, and similarly for the other g_i.

Now $M_i = \mathrm{diag}(\mathbf{r}^i)^{-1} g_i$ is a complex matrix with row sums equal to one. Letting $\boldsymbol{\pi} = (\prod_{i=1}^3 r_1^i, \ldots, \prod_{i=1}^3 r_k^i)$ be the vector of entry-wise products of the $\mathbf{r}^i$, the entries of $\boldsymbol{\pi}$ are nonzero and

$$P = \mathrm{Diag}(\boldsymbol{\pi}) \cdot (M_1, M_2, M_3).$$

Since P is a distribution,

$$\begin{aligned}
1 &= ((P *_1 \mathbf{1}) *_2 \mathbf{1}) *_3 \mathbf{1} \\
&= (((\mathrm{Diag}(\boldsymbol{\pi}) \cdot (M_1, M_2, M_3)) *_1 \mathbf{1}) *_2 \mathbf{1}) *_3 \mathbf{1} \\
&= ((\mathrm{Diag}(\boldsymbol{\pi}) *_1 M_1\mathbf{1}) *_2 M_2\mathbf{1}) *_3 M_3\mathbf{1} \\
&= ((\mathrm{Diag}(\boldsymbol{\pi}) *_1 \mathbf{1}) *_2 \mathbf{1}) *_3 \mathbf{1} \\
&= \boldsymbol{\pi} \cdot \mathbf{1},
\end{aligned}$$

so $\boldsymbol{\pi}$ is a valid complex root distribution. Thus, P is in the image of ψ_T for complex, nonsingular parameters.

The forward implication in the theorem is straightforward.

The uniqueness of nonsingular parameters up to permutation of states at the internal node of the tree was discussed at the end of subsection 2.3. ∎

Combining this Proposition with Theorems 3.1 and 3.2 we obtain the following.

COROLLARY 3.4. *A $k \times k \times k$ complex distribution P is the image of complex, nonsingular parameters for GM(k) on the 3-leaf tree if, and only if, it satisfies the semialgebraic conditions (i) and (ii) of Theorem 3.2 and*

(iii) for $i = 1, 2, 3$, $\det(P *_i \mathbf{1}) \neq 0$.

For $k = 2$, P is the image of real nonsingular parameters for GM(2) on the 3-leaf tree if, and only if, it satisfies $\Delta(P) > 0$ and the semialgebraic conditions (iii).

Next we characterize the image of nonsingular stochastic parameters, and finally of strictly positive nonsingular parameters. The key to this step is the construction of certain quadratic forms whose positive semi-definiteness (respectively definiteness) encodes nonnegativity (respectively positivity) of some of the numerical parameters. Sylvester's Theorem [35], which we state for reference here, then gives a semialgebraic version of these conditions.

Recall that a *principal minor* of a matrix is the determinant of a submatrix chosen with the same row and column indices, and that a *leading* principal minor is one of these where the chosen indices are $\{1, 2, 3, \dots, k\}$ for any k.

THEOREM 3.5 (Sylvester's Theorem). *Let A be an $n \times n$ real symmetric matrix and $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$ the associated quadratic form on $\mathbb{R}^n$. Then*

1. *Q is positive semidefinite if, and only if, all principal minors of A are nonnegative, and*
2. *Q is positive definite if, and only if, all leading principal minors of A are strictly positive.*

We use Sylvester's Theorem to establish the following theorem.

THEOREM 3.6. *A $k \times k \times k$ tensor P is the image of nonsingular stochastic parameters for the GM(k) model on the 3-leaf tree if, and only if, its entries are nonnegative and sum to 1, conditions (i), (ii), and (iii) of Theorem 3.2 and Corollary 3.4 are satisfied, and*

(iv) all leading principal minors of

$$\det(P_{\cdot\cdot+})P_{+\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+})P_{\cdot+\cdot}, \tag{3.2}$$

are positive, and all principal minors of the following matrices are nonnegative:

$$\begin{aligned} &\det(P_{\cdot\cdot+})\, P_{i\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+})P_{\cdot+\cdot}, && \text{for } i = 1, \dots, k, \\ &\det(P_{\cdot\cdot+})P_{+\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+})P_{\cdot i\cdot}, && \text{for } i = 1, \dots, k, \\ &\det(P_{+\cdot\cdot})P_{\cdot+\cdot} \operatorname{adj}(P_{+\cdot\cdot})P_{\cdot\cdot i}^T, && \text{for } i = 1, \dots, k. \end{aligned} \tag{3.3}$$

Moreover, P is the image of nonsingular positive parameters if, and only if, its entries are positive and sum to 1, conditions (i), (ii), and (iii) are satisfied and

(iv') all leading principal minors of the matrices in (3.2) and (3.3) are positive.

In both of these cases, the nonsingular parameters are unique up to label swapping.

Proof. Let P be an arbitrary nonnegative $k \times k \times k$ tensor whose entries sum to 1. By Corollary 3.4, the first 3 conditions are equivalent to $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ for complex nonsingular parameters. We need to show the addition of assumption (iv) is equivalent to parameters being nonnegative.

Note that

$$\begin{aligned} P_{\cdot\cdot+} &= P *_3 \mathbf{1} = M_1^T \operatorname{diag}(\boldsymbol{\pi}) M_2, \\ P_{\cdot+\cdot} &= P *_2 \mathbf{1} = M_1^T \operatorname{diag}(\boldsymbol{\pi}) M_3, \\ P_{+\cdot\cdot} &= P *_1 \mathbf{1} = M_2^T \operatorname{diag}(\boldsymbol{\pi}) M_3. \end{aligned}$$

Since $P_{\cdot\cdot+}$ is nonsingular, we find

$$P_{+\cdot\cdot}^T P_{\cdot\cdot+}^{-1} P_{\cdot+\cdot} = M_3^T \operatorname{diag}(\boldsymbol{\pi}) M_3 \tag{3.4}$$

is symmetric, and the matrix of a positive definite quadratic form if, and only if the entries of $\boldsymbol{\pi}$ are positive. Equivalently, by Sylvester's theorem, all leading principal minors of this matrix must be positive.

Similarly, using slices one has

$$P_{i\cdot\cdot}^T P_{\cdot\cdot+}^{-1} P_{\cdot+\cdot} = M_3^T \operatorname{diag}(\boldsymbol{\pi}) \Lambda_{1,i} M_3$$

where $\Lambda_{1,i} = \operatorname{diag}(M_1 \mathbf{e}_i)$ is the diagonal matrix with entries from the ith column of M_1. Thus its principal minors being nonnegative is equivalent (since we already have that the entries of $\boldsymbol{\pi}$ are positive) by Sylvester's Theorem to the entries in the ith column of M_1 being nonnegative. The product $P_{+\cdot\cdot}^T P_{\cdot\cdot+}^{-1} P_{\cdot i\cdot}$ similarly can be used for a condition that the ith column of M_2 be nonnegative, and the product $P_{\cdot+\cdot} P_{+\cdot\cdot}^{-1} P_{\cdot\cdot i}^T$ for the columns of M_3.

Multiplying all these matrices by the square of an appropriate nonzero determinant clears denominators and preserves signs, yielding (3.2) and (3.3).

For the second statement, that the matrices in (3.2) and (3.3) have positive leading principal minors is equivalent, by Sylvester's Theorem, to the positive definiteness of the quadratic forms, which in turn is equivalent to the positiveness of parameters. Since these parameters are nonsingular, the only source of non-uniqueness is label swapping. ∎

Remark. Matrix products such as that of equation (3.4) appeared in [3], where their symmetry was used to produce phylogenetic invariants, but their usefulness for stating nonnegativity of parameters was overlooked.

Remark. The $j \times j$ minors of the matrices in (3.2) and (3.3) are polynomials in the entries of P of degree $j(2k+1)$, with $j = 1, \dots, k$. However, as the leading determinant in those products is real and nonzero, one can remove an even power of it without affecting the sign of the minors. Thus the polynomial inequality of degree $j(2k+1)$ can be replaced by one of lower degree, $j(k+1) + e_j k$, where $e_j = 0$ or 1 is the parity of j.

In the case of the 2-state model, the above result can be made more complete, by also explicitly describing the image of singular parameters. While semialgebraic characterizations of probability distributions for both nonsingular and singular parameters on the 3-leaf tree have been given previously by [32], [10], [23], and [37], we provide another since our approach is novel.

Theorem 3.7. *A tensor P is in the image of the stochastic parameterization map ψ_T for the GM(2) model on the 3-leaf tree if, and only if, its entries are nonnegative and sum to 1, and one of the following occur:*

1. $\Delta(P) > 0$, $\det(P *_i \mathbf{1}) \neq 0$ *for* $i = 1, 2, 3$*, all leading principal minors of*

$$\det(P_{\cdot\cdot+}) P_{+\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+}) P_{\cdot+\cdot}$$

are positive, and all principal minors of the following six matrices are nonnegative:

$$\det(P_{\cdot\cdot+})\, P_{i\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+})P_{\cdot+\cdot}, \quad \textit{for } i = 1,2,$$
$$\det(P_{\cdot\cdot+})P_{+\cdot\cdot}^T \operatorname{adj}(P_{\cdot\cdot+})P_{\cdot i\cdot}, \quad \textit{for } i = 1,2,$$
$$\det(P_{+\cdot\cdot})P_{\cdot+\cdot} \operatorname{adj}(P_{+\cdot\cdot})P_{\cdot\cdot i}^T, \quad \textit{for } i = 1,2.$$

In this case, P is the image of unique (up to label swapping) nonsingular parameters.

2. $\Delta(P) = 0$*, and all* 2×2 *minors of at least one of the matrices* $\mathrm{Flat}_{1|23}(P)$*,* $\mathrm{Flat}_{2|13}(P)$*,* $\mathrm{Flat}_{3|12}(P)$ *are zero. In this case, P arises from singular parameters. If P has all positive entries, then it is the image of infinitely many singular stochastic parameter choices.*

Proof. Using Theorem 3.6, and the observations made for $k = 2$ immediately following the statement of Theorem 3.2, case 1 is already established under the weaker condition that $\Delta(P) \neq 0$. However, since the parameters are nonsingular and real when $\Delta(P) \neq 0$ and the conditions of case 1 are satisfied, by Theorem 3.1 we may assume equivalently that $\Delta(P) > 0$.

To establish case 2, first assume $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ is the image of singular stochastic parameters. Then certainly P has nonnegative entries summing to 1, and by equations (2.1) and (3.1), $\Delta(P) = 0$. Since

$$\mathrm{Flat}_{1|23}(P) = M_1^T \operatorname{diag}(\boldsymbol{\pi})M,$$

where M is the 2×4 matrix obtained by taking the tensor product of corresponding rows of M_2 and M_3, this flattening has rank 1, if $\boldsymbol{\pi}$ has a zero entry or M_1 has rank 1. Similar products for the other flattenings show that singular parameters imply at least one of the flattenings $\mathrm{Flat}_{1|23}(P), \mathrm{Flat}_{2|13}(P), \mathrm{Flat}_{3|12}(P)$ has rank 1, and hence its 2×2 minors vanish.

Conversely, suppose $\Delta(P) = 0$ and at least one of the flattenings has vanishing 2×2 minors, and hence rank 1. Then by the classification of orbits given in [16, Table 7.1], P is in the $GL(2,\mathbb{R})^3$-orbit of one of the following four tensors: the tensor $\mathrm{Diag}(1,0)$ (in which case all three flattenings have rank 1) or one of the 3 tensors with parallel slices I and the zero matrix (in which case exactly one of the flattenings has rank 1).

If $P = \mathrm{Diag}(1,0)\cdot(g_1, g_2, g_3)$, then $P(i,j,k) = g_1(1,i)g_2(1,j)g_3(1,k)$. Since the entries of P are nonnegative and sum to 1, one sees the top rows of each g_i can be chosen to be nonnegative, summing to 1. The bottom row of each g_i can also be replaced with any nonnegative row summing to 1 that is independent of the top row. Taking $\boldsymbol{\pi} = (1,0)$, this gives us infinitely many choices of singular stochastic parameters giving rise to P. Alternatively, one could choose each Markov matrix to have two identical rows, and any $\boldsymbol{\pi}$ with nonzero entries to obtain other singular stochastic parameters leading to P.

For the remaining cases assume, without loss of generality, that $P = E\cdot(g_1, g_2, g_3)$, where $E_{\cdot\cdot1} = (1/2)\,I$, and $E_{\cdot\cdot2}$ is the zero matrix. Then $P_{\cdot\cdot1} = g_3(1,1)(g_1^T g_2)$ and $P_{\cdot\cdot2} = g_3(1,2)(g_1^T g_2)$. Since the entries of P are nonnegative and add to 1, we may assume that the top row of g_3 is also nonnegative and adds to 1. Choose M_3 to have two identical rows matching the top row of g_3. Now $P_{\cdot\cdot+} = g_1^T g_2$ is a rank-2 nonnegative matrix with entries adding to 1. Such a matrix can be written in the form $P_{\cdot\cdot+} = M_1^T \operatorname{diag}(\boldsymbol{\pi})M_2$ with, for instance $M_1 = I$, $\boldsymbol{\pi} = P_{\cdot++}$, $M_2 = \operatorname{diag}(\boldsymbol{\pi})^{-1}P_{\cdot+\cdot}$. Then one has $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$. If P has positive entries one may also choose

M_1 sufficiently close to I so that M_1, $\boldsymbol{\pi} = (M_1^T)^{-1}P_{\cdot++}$, $M_2 = \operatorname{diag}(\boldsymbol{\pi})^{-1}\left(M_1^T\right)^{-1}P_{\cdot\cdot+}$ all have nonnegative entries, thus obtaining infinitely many singular parameter choices leading to P. (The example of $P = E$ shows that with only nonnegative entries there may be only finitely many singular parameter choices leading to P.) ∎

Remark. The analysis of the singular parameter case in this proof, by appealing without explanation to [16, Table 7.1], has not made explicit the importance of the notion of *tensor rank.* Indeed, that concept is central to both [16] and [1] and thus plays a crucial behind-the-scenes role in this work as well. The first singular case, a tensor in the orbit of $\operatorname{Diag}(1,0)$, is of tensor rank 1, while the second, a tensor in the orbit of E, is of tensor rank 2 yet multlilinear rank $(2,2,1)$. The nonsingular case is those of tensor rank 2 and multlinear rank $(2,2,2)$.

Remark. In case 1 of the theorem, the polynomial inequalities are of degree 4 and 2 (from Δ and the determinants) and degree 5 and 10 (from the minors), but the degree 10 ones can be lowered to degree 6 by removing a factor of a determinant squared. The polynomial equalities appearing in case 2 have degree 4 and 2, with the quadratics simply expressing that one of the leaf variables is independent of the others.

Minor modifications to the argument give the extension to positive parameters below.

THEOREM 3.8. *A tensor P is in the image of the positive stochastic parameterization map for the GM(2) model on the 3-leaf tree if, and only if, its entries are positive and sum to 1, and the conditions of Theorem 3.7 are met with the following modification to case 1: all leading principal minors of the matrices are positive.*

Proof. Case 1 is proved by combining the arguments for Theorems 3.6 and 3.7.

For case 2, if P is in the orbit of $\operatorname{Diag}(1,0)$ the argument of Theorem 3.7 still applies, replacing 'nonnegative' with 'positive', and using the second construction of singular parameters. If P is in the orbit of E we simply replace 'nonnegative' with 'positive' in the argument. ∎

As mentioned above, semialgebraic descriptions of the binary general Markov model on trees have been given previously, but in ways where generalizations to k-state models were not apparent. Although we have considered only the 3-leaf tree (with larger trees to be discussed in §5) thus far, we pause here to discuss some connections to the recent works of Zwiernik and Smith [37] and Klaere and Liebscher [23] on semialgebraic descriptions of the binary model on trees, as well as the older work of Pearl and Tarsi [29].

Though using different approaches (and in the case of [29] with different goals), all three of these works emphasize statistical interpretations of various quantities computed from a probability distribution P (*e.g.*, covariances, conditional covariances, moments, tree cumulants). While analogs of some of the same quantities appear in our generalization to k-state models, we have used algebra, rather than statistics, to guide our derivation. Although an inequality such as $\det(P *_i \mathbf{1}) \neq 0$ which appears in our description can be given a simple statistical interpretation when $k = 2$ (that two leaf variables are not independent), for larger k its meaning is more subtle, as it is tied to our notion of nonsingular parameters. Thus our generalization to k-state models uses a more detailed development than the simple generalization of statistical concepts from $k = 2$ to larger k.

The role played by the hyperdeterminant Δ in giving a semialgebraic model description for $k = 2$ was first made clear in [37]. Its role was essentially independently discovered in [23, Theorem 6], though without recognition that it is a classical algebraic object. Indeed, both works recognize Δ as an expression in the 2-variable and 3-variable covariances (*i.e.*, central moments). This is a fascinating intertwining of algebra and statistics, yet we did not find it helpful in understanding the correct analog of Δ for higher k; rather, [1] develops the analog f_i used here through algebraic motivation entirely. It would nonetheless be interesting to understand whether f_i can be described in more statistical language.

The explicit semialgebraic model descriptions for the 2-state model given in both [37] and [23] take on quite different forms than ours. This is not a surprise as such a description is far from unique, and different reasoning may produce different inequalities. The version in [37], for example, is stated in a different coordinate system, using tree cumulants rather than the entries of P. We find all these descriptions valuable, as what should be considered the simplest, or most natural, description is not obvious.

The focus of [29] is on recovery of parameters for GM(2) on the 3-leaf tree from a probability distribution assumed to have arisen from stochastic parameters, in an approach based on earlier work in latent structure analysis [27]. In addressing this question, however, semialgebraic conditions on the distribution are obtained. For instance, the non-vanishing of denominators is needed for formulas to make sense, and thus certain polynomials must be nonzero. (The authors seem to assume nonsingularity of parameters, though that is never clarified in the paper.) While Δ never arises in [29], it is remarkable to note, then, that using the results of Theorem 3.1 and making explicit the tacit assumptions that various rational expressions exist and are real, the conditions given in Theorem 1 of [29] are sufficient to show $\Delta(P) > 0$, and thus P is in the image of stochastic nonsingular parameters. Thus one can extract a semialgebraic model description from this work, even if that was not its goal.

4. Inequalities for 3-leaf trees via Sturm theory. The semialgebraic model descriptions given in the previous section have the advantage of being easily describable in a uniform way for all k. However, semialgebraic descriptions are not unique, and there is no clear notion of what description should be considered simplest. It is also of interest, therefore, to obtain alternative polynomial inequalities, possibly of lower degree, that must also be satisfied by probability distributions in the model, in the hopes that they lead to another, perhaps better, semialgebraic model description, or that they might be of further use for testing whether a distribution arises from the model. We explore another approach to doing so here.

4.1. Review of Sturm Theory. Sturm theory can be used to impose conditions that roots of a univariate polynomial lie in a certain interval. We briefly recall basic definitions and results. Suppose that $f(x) \in \mathbb{R}[x]$ is a non-constant polynomial of degree m, with no multiple roots, and we wish to count the roots of f in an interval (a, b) where $f(a)f(b) \neq 0$. Then a *Sturm sequence* $\mathcal{S}$ for f on the interval $[a, b]$ is a sequence $f = f_0, f_1, \dots, f_m$ of polynomials satisfying certain sign relationships at the zeros of the f_j in the interval $[a, b]$. We give an example below, but for specifics, see, for instance, [22]. For any $c \in [a, b]$ which is not a root of any f_i, the *sign variation* $V_S(c)$ is the number of sign changes in the sequence $f(c), f_1(c), \dots, f_m(c)$.

Theorem 4.1 (Sturm's Theorem). *Let $f(x) \in \mathbb{R}[x]$ be a non-constant polynomial and $\mathcal{S}$ a Sturm sequence for f on $[a, b]$. Then the number of distinct roots of $f(x)$ in (a, b) is equal to $V_{\mathcal{S}}(a) - V_{\mathcal{S}}(b)$.*

Though other constructions of Sturm sequences exist, we use the *standard sequence*, derived using a modified Euclidean algorithm. If $f = f_0$ is a polynomial of degree $m > 0$, then set $f_1 = f'$, and for $j = 2, \dots, m$, take f_j to be the opposite of the remainder of division of f_{j-2} by f_{j-1}. This yields a Sturm sequence for f on any interval $[a,b]$ with $f_j(a) \neq 0$, $f_j(b) \neq 0$.

To illustrate, suppose that $f(x) = x^2 + c_1 x + c_0 \in \mathbb{R}[x]$. Then the standard sequence is $f, 2x + c_1, \frac{c_1^2}{4} - c_0$. For the particular choice of coefficients $c_1 = -\frac{3}{4}$ and $c_0 = \frac{1}{8}$, using this sequence on $[0,1]$, we calculate that $f_0(0), f_1(0), f_2(0)$ is the sequence $\frac{1}{8}, -\frac{3}{4}, \frac{1}{64}$, and $f_0(1), f_1(1), f_2(1) = \frac{3}{8}, \frac{5}{4}, \frac{1}{64}$. Thus, $V_{\mathcal{S}}(0) = 2$, $V_{\mathcal{S}}(1) = 0$, so f has $V_{\mathcal{S}}(0) - V_{\mathcal{S}}(1) = 2$ roots in $(0,1)$. Indeed, the factorization $f(x) = \left(x - \frac{1}{2}\right)\left(x - \frac{1}{4}\right)$ shows this directly.

Two comments are in order: First, in this example observe that $f_2(x)$ is one-fourth the discriminant of $f(x)$, and its positivity ensures that a monic quadratic has distinct and real roots. This shows that Sturm theory can produce familiar algebraic expressions, such as the quadratic discriminant, and thus gives a tool for generalizing them. The second observation we state more formally, as it is needed in our arguments below.

Corollary 4.2. *If $f(x)$ is of degree m with neither 0 nor 1 a root, and S is a Sturm sequence for f on $[0,1]$, then f has m distinct roots in this interval precisely when $V_{\mathcal{S}}(0) = m$ and $V_{\mathcal{S}}(1) = 0$.*

This corollary allows us to obtain inequalities ensuring a polynomial has distinct roots in $[0,1]$: One simply requires that the $f_i(0)$ alternate in being > 0 or < 0, while the $f_i(1)$ either be all > 0 or all < 0. We informally refer to inequalities obtained in this manner as *Sturm sequence inequalities.*

4.2. Eigenvalues and Sturm Sequences. We now give a second construction of inequalities that, if satisfied, ensure that GM(k) model parameters on a 3-leaf tree are stochastic. While in §3 we constructed matrices encoding positivity of parameters through requirements on associated quadratic forms, here we instead construct matrices whose eigenvalues encode parameters.

Suppose that $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ for complex nonsingular $\{\boldsymbol{\pi}, M_1 M_2, M_3\}$. Recall that for $i \in [k]$,

$$P_{i\cdot\cdot} = P *_1 \mathbf{e}_i = M_2^T \operatorname{diag}(\boldsymbol{\pi}) \Lambda_{1,i} M_3,$$
$$P_{+\cdot\cdot} = P *_1 \mathbf{1} = M_2^T \operatorname{diag}(\boldsymbol{\pi}) M_3$$

where $\Lambda_{1,i} = \operatorname{diag}(M_1 \mathbf{e}_i)$ is the diagonal matrix with entries from the ith column of M_1. Thus, by nonsingularity of the parameters,

$$A_{1,i} := P_{+\cdot\cdot}^{-1} P_{i\cdot\cdot} = M_3^{-1} \Lambda_{1,i} M_3$$

has as eigenvalues the entries of the ith column of M_1. (This construction underlies the proof of parameter identifiability for the GM(k) model on trees [15], and the construction of phylogenetic invariants in [3], including the equality in condition (i) of Theorem 3.2 of this paper.) Similarly we define the matrices

$$A_{2,i} := P_{\cdot+\cdot}^{-1} P_{\cdot i\cdot} = M_3^{-1} \Lambda_{2,i} M_3,$$
$$A_{3,i} := P_{\cdot\cdot+}^{-1} P_{\cdot\cdot i} = M_2^{-1} \Lambda_{3,i} M_2$$

with $\Lambda_{j,i} = \operatorname{diag}(M_j \mathbf{e}_i)$ the diagonal matrix with entries from the ith column of the matrix M_j.

Proposition 4.3. *Let $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ be a real $k \times k \times k$ tensor that is the image of complex nonsingular parameters. For each of the matrices $A_{j,i}$,*

$j \in \{1,2,3\}$, $i \in [k]$, assume the characteristic polynomial has neither 0 nor 1 as a root, and let $\mathcal{S}_{j,i}$ denote the standard Sturm sequence for it. Then $V_{\mathcal{S}_{j,i}}(0) = k$ and $V_{\mathcal{S}_{j,i}}(1) = 0$ for all i, j if, and only if, the matrices M_1, M_2, M_3 are positive Markov matrices with no repeated element in any column and $\boldsymbol{\pi}$ is real.

Proof. The statement about the M_i follows from Corollary 4.2. Then, since the M_i are real and invertible

$$\boldsymbol{\pi} = ((P \cdot (M_1^{-1}, M_2^{-1}, M_3^{-1})) *_1 \mathbf{1}) *_2 \mathbf{1}$$

shows $\boldsymbol{\pi}$ is real. ∎

Each matrix $A_{j,i}$ has entries that are rational in the entries of P, with denominator $\det(P *_j \mathbf{1})$ of degree k and numerator of degree k. The characteristic polynomial f of $A_{j,i}$ thus also has coefficients that are rational functions in P, and in fact the non-leading coefficients c_i of f are rational of degree k over k. This can be seen explicitly, for example when $j = 1$, in the following:

$$\begin{aligned} f(x) &= \det(xI - P_{+\cdot\cdot}^{-1} P_{i\cdot\cdot}) \\ &= \det(x P_{+\cdot\cdot}^{-1} P_{+\cdot\cdot} - P_{+\cdot\cdot}^{-1} P_{i\cdot\cdot}) \\ &= \det\left(P_{+\cdot\cdot}^{-1}(x P_{+\cdot\cdot} - P_{i\cdot\cdot})\right) \\ &= \frac{\det\left(x P_{+\cdot\cdot} - P_{i\cdot\cdot}\right)}{\det(P_{+\cdot\cdot})}. \end{aligned} \tag{4.1}$$

It follows that the Sturm sequence inequalities, which are constructed from the coefficients c_i, are rational in the entries of P as well. Indeed, by multiplying each of these inequalities by a sufficiently high even power of $\det(P *_j \mathbf{1})$ to avoid changing signs, these expressions become polynomial in P. Thus, one can phrase the conditions $V_{\mathcal{S}_{j,i}}(0) = k$ and $V_{\mathcal{S}_{j,i}}(1) = 0$ as a collection of polynomial inequalities. Finally, note that since f is a monic characteristic polynomial, then $(-1)^k f_0(0) = \det(A_{j,i}) > 0$ and $f_k(0) = f_k(1)$, so the signs of all $f_j(0)$ and $f_j(1)$ are determined. This leads to the following:

Corollary 4.4. *Consider real $k \times k \times k$ tensors $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ arising from complex nonsingular parameters. Then one can give a finite collection of strict polynomial inequalities that hold precisely when the M_i are positive Markov matrices with no repeated column entries, and $\boldsymbol{\pi}$ is real.*

Remark. For simplicity, we have restricted our discussion to polynomials with no multiple roots, leading to the constraints on the matrix column entries given above. However, this restriction can be removed, by considering Sturm sequences for polynomials with repeated roots. We suggest [24, 28] for futher information.

Note that the non-strict versions of the inequalities of Corollary 4.4 must continue to hold on the closure of the image of parameters described in the corollary. As this closure includes the image of Markov matrices which may have repeated column entries, or entries of 0 or 1, or are singular, the non-strict inequalities hold for *all* stochastic parameters.

However, some distributions arising from non-stochastic parameters may satisfy the non-strict inequalities as well. Thus while we have obtained semialgebraic statements guaranteeing stochasticity of nonsingular parameters of a particular form, this does not seem to lead to a complete semialgebraic description of the image of all stochastic parameters for arbitrary k. In the case $k = 2$, however, we can do better, as we show next.

4.3. Sturm sequences for GM(2). In the specific case of the 2-state model, we explicitly give the inequalities of Corollary 4.4. To this end, suppose that $P = \psi_T(\boldsymbol{\pi}, \{M_1, M_2, M_3\})$ is a $2 \times 2 \times 2$ probability distribution arising from nonsingular parameters.

For any $j \in \{1, 2, 3\}$, $i \in [2]$, let $A = A_{j,i}$. The standard Sturm sequence of the characteristic polynomial of A is

$$\begin{aligned} f_0 &= t^2 - \mathrm{tr}(A)t + \det(A), \\ f_1 &= 2t - \mathrm{tr}(A), \\ f_2 &= \frac{1}{4}(\mathrm{tr}(A)^2 - 4\det(A)) = \frac{1}{4}\delta(f_0), \end{aligned}$$

where $\delta(f)$ denotes the discriminant of the monic quadratic polynomial f.

Since $k = 2$, the nonsingularity of the M_i together with the fact that their rows sum to 1 implies that none of their columns have repeated entries. Thus the characteristic polynomial f_0 must have distinct roots. To ensure that these roots are in $(0, 1)$, so that the matrix parameters are Markov, the variation in signs of the Sturm sequence must be:

$$\begin{aligned} f_0(0) &= \det(A) > 0, & f_0(1) &= 1 - \mathrm{tr}(A) + \det(A) > 0, \\ f_1(0) &= -\mathrm{tr}(A) < 0, & f_1(1) &= 2 - \mathrm{tr}(A) > 0, \\ f_2(0) &= \frac{1}{4}\delta(f) > 0, & f_2(1) &= \frac{1}{4}\delta(f) > 0. \end{aligned} \tag{4.2}$$

Each of these inequalities can be expressed using rational expressions in the entries of P. For instance, for $j = 1$, $i = 1$, the first two inequalities ensuring that the first column of M_1 has distinct entries between 0 and 1 are

$$f_0(0) = \det(A) = \frac{\det(P_{1\cdot\cdot})}{\det(P_{+\cdot\cdot})} > 0, \tag{4.3}$$

and

$$f_1(0) = -\mathrm{tr}(A) = \frac{-2\det(P_{1\cdot\cdot}) + p_{112}p_{221} - p_{211}p_{122} - p_{111}p_{222} + p_{212}p_{121}}{\det(P_{+\cdot\cdot})} < 0.$$

After multiplying each of the inequalities of (4.2) by $\det(P_{+\cdot\cdot})^2$ to clear denominators, we obtain five distinct polynomial inequalities of degree 4 in the entries of P, as well as one degree-2 inequality

$$\det(P_{+\cdot\cdot}) \neq 0.$$

Note too that $f_2(0) = f_2(1)$ is a positive multiple of the discriminant of f_0, and its positivity guarantees (again) that the roots of f_0 are distinct and real.

The inequality (4.3) has a direct statistical interpretation: Assuming the states of the variables X_i are encoded with numerical values s and $s + 1$, then $\det(P_{+\cdot\cdot}) = \mathrm{Cov}(X_2, X_3)$ and $\det(P_{1\cdot\cdot})$ is a positive multiple of $\mathrm{Cov}(X_2, X_3 \mid X_1 = 1)$. Thus the inequality states that the sign of the association of X_2 and X_3 is the same whether we have information about X_1 or not. Viewing the 3-leaf tree as a graphical model for nonsingular parameters, this should be expected, but that it arises cleanly from Sturm theory is a pleasant surprise.

Of additional interest is the observation that f_2 can be expressed in terms of the hyperdeterminant $\Delta(P)$:

$$f_2 = \frac{\delta(f)}{4} = \frac{\Delta(P)}{4\det(P_{+\cdot\cdot})^2}.$$

Since $\Delta(P) \neq 0$ implies $\det(P_{+\cdot\cdot}) \neq 0$, we find

$$f_2 > 0 \text{ if, and only if, } \Delta(P) > 0. \tag{4.4}$$

In particular, using Theorem 3.1, we see the Sturm inequality involving f_2 implies that P arises from nonsingular real parameters, and thus an additional assumption of that fact is not needed to supplement the Sturm inequalities.

We further note that the inequalities (4.2) for various $A_{j,i}$ are not independent of one another. Since $A_{j,1} + A_{j,2} = I$, it follows that the two matrices $A_{j,1}$, $A_{j,2}$ give rise to the same inequalities.

The inequalities (4.2), unfortunately, are not sufficient to ensure the root distribution $\boldsymbol{\pi}$ is also positive. For instance,

$$P = \left[\begin{array}{cc|cc} 0.65439 & 0.07191 & 0.16361 & 0.01809 \\ 0.07191 & 0.00079 & 0.01809 & 0.00121 \end{array}\right]$$

is a probability distribution that satisfies $\Delta(P) > 0$ and the Sturm inequalities for each $A_{j,i}$, but the root distribution $\boldsymbol{\pi} = (1.01, -0.01)$ is not stochastic.

Nonetheless, in the 2-state case we can construct another inequality in P that ensures the root distribution is positive. If $P \in \operatorname{Im}(\psi_T)$ for nonsingular real parameters, then

$$\frac{\det(P_{+\cdot\cdot})\det(P_{\cdot+\cdot})\det(P_{\cdot\cdot+})}{\Delta(P)} = \pi_1\pi_2.$$

This is easily verified using transformation properties of the determinants and Δ under the action of (M_1, M_2, M_3) on $\operatorname{Diag}(\boldsymbol{\pi})$. (See [6, p. 136] for an earlier derivation and application of this equation.) Since $\pi_1 + \pi_2 = 1$, the positivity of the π_i is equivalent to

$$0 < \frac{\det(P_{+\cdot\cdot})\det(P_{\cdot+\cdot})\det(P_{\cdot\cdot+})}{\Delta(P)} < \frac{1}{4}.$$

Moreover, because $\Delta(P) > 0$, this in turn is equivalent to the inequalities

$$0 < \det(P_{+\cdot\cdot})\det(P_{\cdot+\cdot})\det(P_{\cdot\cdot+}) < \frac{1}{4}\Delta(P). \tag{4.5}$$

Although the second inequality here is not homogeneous, it can be made homogeneous of degree 6 by multiplication of the right side by $1 = (\sum_{i,j,k=1}^{2} P_{ijk})^2$.

Putting this all together, we have an alternative semialgebraic test, to be contrasted with case 1 of Theorem 3.8, for testing that $\boldsymbol{\pi}$ is stochastic.

Proposition 4.5. *The image of the positive nonsingular parameterization map for GM(2) on a 3-leaf tree can be characterized as the probability distributions satisfying an explicit collection of strict polynomial inequalities:* 3 *of degree* 2, 13 *of degree* 4, *and* 2 *of degree* 6.

Proof. By the above discussion, the degree-2 inequalities $\det(P *_i \mathbf{1}) \neq 0$ and the 5 degree-4 inequalities arising from (4.2) for each of the 3 choices of j suffice to ensure that nonsingular parameters exist, with Markov matrices having positive entries. Only 13 of these degree-4 inequalities are distinct, as each j leads to $\Delta(P) > 0$. Then the degree-6 inequalities of (4.5) ensure $\boldsymbol{\pi}$ has positive entries. ∎

Note that case 1 of Theorem 3.8 gave a description using 3 degree-2, 1 degree-4, 4 degree-5, and 4 degree-6 polynomials. The description arising from Sturm theory thus uses fewer degree-5 and 6 polynomials, but more degree-4 ones.

4.4. Sturm sequences for GM(3). We now give several examples of Sturm sequence inequalities for GM(3) on the 3-taxon tree.

If A is a 3×3 matrix with positive determinant and characteristic polynomial $f(x) = x^3 + c_2 x^2 + c_1 x + c_0$ without roots at 0 or 1, then A has 3 distinct eigenvalues in the interval (0,1) if, and only if,

$$\begin{aligned}
&f_0(0) = c_0 && < 0, \quad && f_0(1) = 1 + c_2 + c_1 + c_0 && > 0,\\
&f_1(0) = c_1 && > 0, \quad && f_1(1) = 3 + 2c_2 + c_1 && > 0,\\
&f_2(0) = -c_0 + \frac{1}{9}c_1c_2 && < 0, \quad && f_2(1) = -\frac{2}{3}c_1 + \frac{2}{9}c_2^2 - c_0 + \frac{1}{9}c_1c_2 && > 0,\\
&f_3(0) = \frac{9}{4}\frac{\delta(f)}{(3c_1 - c_2^2)^2} && > 0, \quad && f_3(1) = \frac{9}{4}\frac{\delta(f)}{(3c_1 - c_2^2)^2} && > 0,
\end{aligned} \tag{4.6}$$

where $\delta(f)$ denotes the discriminant of f. Here, of course, $c_0 = -\det(A)$, $c_2 = -\mathrm{tr}(A)$ and c_1 is quadratic in the entries of A. However, by (4.1), if $A = A_{j,i}$ then each c_i is rational in the entries of P, with numerator of degree 3 and denominator $\det(P *_j \mathbf{1})$.

By multiplying the top 6 inequalities of (4.6) by $\det(P *_j \mathbf{1})^2$, we obtain six polynomial inequalities of degree 6 in P. In the case that $A = A_{1,1} = P_{+\cdot\cdot}^{-1} P_{1\cdot\cdot}$, for example, the first inequality is

$$0 < -\det(P_{+\cdot\cdot})^2 f_0(0) = \det(P_{+\cdot\cdot}) \det(P_{1\cdot\cdot}).$$

By (4.1) we know that $\det(P_{+\cdot\cdot})^2 c_1$ and $\det(P_{+\cdot\cdot})^2 c_2$ are polynomials of the form $\det(P_{+\cdot\cdot})K$, where K is homogeneous of degree 3 in the entries of P. Computations with Maple show K has 42 monomial summands for c_1, and 114 monomial summands for c_2.

The inequality of the bottom row of (4.6) can be simplified to $\delta(f) > 0$, which is of degree 4 in the c_i. Thus, $\det(P_{+\cdot\cdot})^4 \delta(f) > 0$ is a polynomial inequality of degree 12 in P. We omit writing these Sturm inequalities explicitly.

Instead, we illustrate a more direct application of the relevent Sturm theory, in which the semialgebraic description of the model is present only implicitly. Consider the probability distribution with exact rational entries given by

$$P = \left[\begin{array}{ccc|ccc|ccc}
0.1500 & 0.0130 & 0.105\bar{3} & 0.0130 & 0.0050 & 0.015\bar{3} & 0.105\bar{3} & 0.015\bar{3} & 0.077\bar{6}\\
0.0130 & 0.0050 & 0.015\bar{3} & 0.0050 & 0.0090 & 0.009\bar{3} & 0.015\bar{3} & 0.009\bar{3} & 0.018\bar{6}\\
0.105\bar{3} & 0.015\bar{3} & 0.077\bar{6} & 0.015\bar{3} & 0.009\bar{3} & 0.018\bar{6} & 0.077\bar{6} & 0.018\bar{6} & 0.0620
\end{array}\right]. \tag{4.7}$$

One can check that P satisfies the conditions of Theorem 3.2, so P is in the image of nonsingular complex parameters. Then the values of the Sturm sequence at $x = 0$ and $x = 1$ for the characteristic polynomial of $A_{1,1}$ are approximately as in Table 4.1. Thus the sign variations are $V_{\mathcal{S}}(0) = 2$ and $V_{\mathcal{S}}(1) = 1$, so the first column of M_1 has exactly 1 distinct real entry. This then implies that either M_1 is not real, or that its first column contains the same entry in all rows. Since the second possibility implies that a 3×3 Markov matrix is singular, we can conclude that P does not arise from stochastic parameters.

	$f_0(x)$	$f_1(x)$	$f_2(x)$	$f_3(x)$
$x=0$	-0.1087	0.7225	-0.0117	-0.0283
$x=1$	0.1138	0.7225	0.0067	-0.0283

Table 4.1
Sturm sequence values for the characteristics polynomial of $A_{1,1}$ for the tensor P of (4.7)

This example did not actually require the full strength of Sturm's theorem; it is sufficient to note that the discriminant of the cubic characteristic polynomial is negative to conclude that the first column of M_1 has two complex entries, and one real one. This is special to the small size of the state space, however. For the case of most interest in phylogenetics, $k = 4$, the sign of the quartic discriminant alone does not carry enough information to determine whether all roots of a polynomial are real. Moreover, even for $k = 3$, the Sturm sequence is needed to ensure roots are between 0 and 1.

One might optimistically hope that some $k = 3$ analog of the hyperdeterminant, such as those in [1], might arise easily from Sturm theory, as the hyperdeterminant itself did in the case $k = 2$. Unfortunately this does not appear to be the case, at least by the most straightforward considerations.

In closing, we note that for $k \geq 3$ we have not given in this section any condition to ensure that $\boldsymbol{\pi}$ has positive entries. For $k = 2$ we did do so, using the transformation formula for $\Delta(P)$, but this idea does not seem to generalize. The only way we know to obtain a semialgebraic condition ensuring this is through the quadratic form approach used in §3.

5. GM(k) on n-leaf trees. We now extend the results of the previous sections to n-leaf trees, for $n > 3$. To vary the choice of the root node of the tree in our arguments, we need the following. Similar lemmas are given in [33, Theorem 2] and [3, Proposition 1].

Lemma 5.1. *Suppose stochastic parameters are given for the GM(k) model on a tree T with the root located at a specific node of T. Then there are stochastic parameters for T rooted at any other node of T, or at a node of valence* 2 *introduced along an edge of T, which lead to the same distribution. Moreover, if the original parameters were nonsingular and/or positive, then so are the new ones.*

Proof. It is enough to show this on a tree with a single edge, as one may then successively apply that result along the edges in a path in a larger tree.

We show first that the root may be moved from one vertex of an edge to the other. For this it is sufficient to show that given any probability distribution $\boldsymbol{\pi}$ and Markov matrix M, there exists a probability distribution $\tilde{\boldsymbol{\pi}}$ and Markov matrix $\widetilde{M}$ with $\operatorname{diag}(\boldsymbol{\pi})M = P = \widetilde{M}^T \operatorname{diag}(\tilde{\boldsymbol{\pi}})$. This is straightforward if the column sums of P are nonzero. If a column sum of P is zero, and hence all entries in the column are zero, then the corresponding entry of $\tilde{\boldsymbol{\pi}}$ must be zero while that row of $\widetilde{M}$ can be arbitrary. If the original parameters were nonsingular or positive, then showing that the new ones are as well is straightforward.

If instead we wish to move the root from vertex a on edge (a, b) to a new internal node r introduced to subdivide the edge, first introduce r and let $M_{(a,r)} = M_{(a,b)}$

and $M_{(r,b)} = I$. Then move the root from a to r as above. For the case of positive parameters, instead pick $M_{(r,b)}$ to have positive entries but be near enough to I that $M_{(a,r)} = M_{(a,b)}M_{(r,b)}^{-1}$ has positive entries. $\square$

Note that for real or complex parameters Lemma 5.1 fails to hold as the examples $\boldsymbol{\pi} = (1/2, 1/2)$, $M = \begin{pmatrix} s & 1-s \\ 2-s & s-1 \end{pmatrix}$, $s \neq 1$ show. (The problem is simply that a column sum of $\operatorname{diag}(\boldsymbol{\pi})M$ can be zero though the column is not the zero vector.) However, if the parameters are nonsingular, we can still move the root by modifying the above argument. Indeed, nonsingularity of parameters implies that from $\operatorname{diag}(\boldsymbol{\pi})M = \widetilde{M}^T \operatorname{diag}(\tilde{\boldsymbol{\pi}})$ one can solve for a nonsingular $\widetilde{M}$, since the other three matrices in the equation are nonsingular. This shows the following.

LEMMA 5.2. *Suppose real or complex nonsingular parameters are given for the GM(k) model on a tree T with the root located at a specific node of T. Then there are nonsingular parameters for T rooted at any other node of T, or at a node of valence 2 introduced along an edge of T, which lead to the same distribution.*

We now show that independent subsets of variables allow the question of determining if a distribution arises from parameters on a tree to be 'decomposed' into the same question for the marginalizations to the subsets.

PROPOSITION 5.3. *Let P be a joint distribution of a set L of k-state variables such that for some partition $L_1|L_2|\cdots|L_s$ of L, the variable sets L_i and L_j are independent for all $i \neq j$. Suppose the marginal distribution of each L_i arises from nonsingular GM(k) parameters on a tree T_i. Then P arises from GM(k) parameters on any tree T which can be obtained by connecting the trees $T_1, T_2, \dots, T_s$ by the introduction of new edges between them (with endpoints possibly subdividing either edges of the T_i or previously introduced edges joining some of the T_i).*

Note that the converse of this statement, that if P arises from parameters for the GM(k) model on an $|L|$-leaf tree then the marginal distributions of each L_i arise from parameters for the GM(k) model on an $|L_i|$-leaf tree, is well-known, and does not require the independence of the variable sets, or nonsingularity of parameters.

Proof. It is enough to consider a partition of L into two independent subsets, $L_1|L_2$. Let T be any tree formed by connecting T_1 and T_2 by a single edge, possibly with endpoints introduced to subdivide edges of one or both of the T_i. If $e = (r_1, r_2)$ is the edge joining T_1 and T_2, with r_i in T_i, then by Lemma 5.2 we may assume that parameters on T_1 and T_2 are given for roots r_1 and r_2. We root T at r_1 and then specify parameters on T as the root distribution $\boldsymbol{\pi}_1$ for T_1, all matrix parameters on the edges of T_1 and T_2, and for the edge e the matrix $M_e = \mathbf{1}\boldsymbol{\pi}_2{}^T$ where $\boldsymbol{\pi}_2$ is the root distribution on T_2.

Let $\tilde{P}$ denote the image of these parameters under ψ_T. The edge e of T induces the split $L_1|L_2$ of the leaf variables, and flattening with respect to e gives $\operatorname{Flat}_e(\tilde{P}) = A^T CB$ where A, B are $k \times k^{|L_1|}$ and $k \times k^{|L_2|}$ matrices depending only on the matrix parameters on the subtrees T_1 and T_2, and

$$\begin{aligned} C &= \operatorname{diag}(\boldsymbol{\pi}_1)M_e, \\ &= \operatorname{diag}(\boldsymbol{\pi}_1)\mathbf{1}\boldsymbol{\pi}_2^T = \boldsymbol{\pi}_1\boldsymbol{\pi}_2^T. \end{aligned}$$

Indeed, in the stochastic case, A gives probabilities of observations at the leaves L_1 conditioned on the state at r_1, B gives probabilities of observations at the leaves L_2 conditioned on the state at r_2, and C is a matrix giving the joint distribution of states at r_1 and r_2. Observing that $A^T CB = (A^T\boldsymbol{\pi}_1)(\boldsymbol{\pi}_2^T B)$, independence implies that $\tilde{P}$ is the product of the same marginal distributions on L_1 and L_2 as P, and hence $\tilde{P} = P$. $\square$

One can replace the assumption of nonsingularity of parameters in this proposition with one of stochasticity, since the main technical point in the proof is that we need freedom to move the root to any node of valence 2 along an edge of T. By Lemma 5.1, this holds for stochastic parameters, so we obtain the following.

Proposition 5.4. *With P and the L_i as in Proposition 5.3, if the marginal distributions of each L_i arise from stochastic parameters for the GM(k) model on an $|L_i|$-leaf tree, then P arises from stochastic parameters for the GM(k) model on an $|L|$-leaf tree. If the parameters on the $|L_i|$-leaf trees are positive, so are those on the $|L|$-leaf tree.*

By this proposition, the only sets we must understand to build a semialgebraic description for the full n-leaf stochastic model are the image of parameters for m-leaf trees, $m \leq n$, when no subsets of the m leaf variables are independent. In the case $k = 2$, by Proposition 2.2, this is precisely the images of nonsingular parameters. Unfortunately, for larger k characterizing such images is much more difficult, and we do not accomplish it in this paper.

One way to think about the difficulty with $k > 2$ is in terms of matrix rank. When $k = 2$, a Markov matrix has either rank 1 or rank 2, which results in independent variables or nonsingular parameters, respectively. For larger k, a Markov matrix may have rank between the extremes of 1 and k, which again produce independent variables or nonsingular parameters. These intermediate cases of singular Markov matrices that are not of rank 1 would each require a detailed analysis, both in the 3-leaf tree case, and then to produce some type of decomposition for larger trees.

Rather than pursue a detailed semialgebraic model description allowing all ranks of Markov matrices for all k, we instead choose to focus on the image of nonsingular parameters. These are certainly the most important in most applications. Moreover, any distribution arising from singular parameters will lie in the topological closure of this set, as singular parameters can be approximated by nonsingular ones. Of course the closure may also contain points that do not arise from any parameters, so this does not circumvent the difficulties of dealing with the many special cases of intermediate rank if an exact semialgebraic description of the full stochastic model is desired.

In the setting of nonsingular, though not necessarily stochastic parameters, we obtain the following.

Proposition 5.5. *Let P be an n-dimensional $k \times k \times \cdots \times k$ distribution with $n \geq 3$. Then P arises from nonsingular complex parameters on a binary tree T if, and only if,*

(i) *All marginalizations of P to 3 variables arise from nonsingular parameters on the induced 3-leaf, 3-edge trees, and*

(ii) *For all internal edges e of T, all $(k+1) \times (k+1)$ minors of the matrix flattening $Flat_e(P)$ are 0.*

Moreover, such nonsingular parameters are unique up to label swapping at internal nodes of T.

Note that condition (i) can be stated in terms of explicit semialgebraic conditions, using Corollary 3.4. Also, the polynomial equalities of condition (ii) are usually called *edge invariants* [8].

Proof. For the forward implication, condition (i) follows since marginalizations arise from the model on the associated induced subtree, using Markov matrices that are products of the original ones. Item (ii) is from [8], where it is shown that all $P \in \mathrm{Im}(\psi_T)$ satisfy the edge invariants. (The nonsingularity of parameters is not required for either of these.)

For the reverse implication, we proceed by induction on the size n of the variable set L. The claim holds by assumption in the base case of $n = 3$. Assume the statement is true for fewer than $n \geq 4$ variables. We identify leaves of T with the variables associated to them. Choose some internal edge $e_0 = (a, b)$ of T, corresponding to the split $L_1|L_2$ of L, with $|L_1|, |L_2| \geq 2$, a in the subtree spanned by L_1, and b in the subtree spanned by L_2. Introducing a vertex c subdividing (a, b), let T_1 be the subtree with leaves $L_1 \cup \{c\}$ and T_2 the subtree with leaves $L_2 \cup \{c\}$. Thus (a, c) in T_1 and (b, c) in T_2 are the edges formed from dividing (a, b).

Since the edge invariants are satisfied by P, $\mathrm{Flat}_{e_0}(P)$ has rank at most k. Therefore, there exist $k^{|L_1|} \times k$ and $k \times k^{|L_2|}$ matrices A, B, both of rank at most k, with

$$\mathrm{Flat}_{e_0}(P) = AB.$$

Choose a single variable $\ell_2 \in L_2$ and let Q denote the marginalization of P to $L_1 \cup \{\ell_2\}$. Then there is a $k^{|L_2|} \times k$ matrix N such that

$$\mathrm{Flat}_{e_0}(P)N = ABN = \mathrm{Flat}_{e_1}(Q),$$

where this last flattening is along the edge $e_1 = (a, \ell_2)$ in the induced subtree on $L_1 \cup \{\ell_2\}$. Stated differently, multiplication by N marginalizes over all those leaves in L_2 except ℓ_2.

Since Q also satisfies conditions (i) and (ii), by the inductive hypothesis Q arises from nonsingular parameters. Moreover, we see that $\mathrm{Flat}_{e_1}(Q)$ has rank k, since marginalization over all but one variable in L_1 is seen to produce a rank k matrix from the nonsingular parameterization. It follows that the $k \times k$ matrix BN has rank k. Replacing A and B with AC and $C^{-1}B$ for some invertible $k \times k$ matrix C, we may further assume the rows of BN add to 1.

Now since Q arises from nonsingular parameters on a $(|L_1|+1)$-leaf tree isomorphic to T_1 rooted at a, we claim that $Q' = Q *_{\ell_2} (BN)^{-1}$ arises from nonsingular complex parameters on T_1 for some suitable choice of B. Indeed, Q' arises from the same parameters as Q, except that on the edge (a, c) we use the matrix parameter that is the product of the one on the edge leading to ℓ_2 and $(BN)^{-1}$. Since $(BN)^{-1}$ is a nonsingular matrix with rows summing to one, the only condition to check is that the marginalization of the resulting distribution to c has no zero entries. But this marginalization is $\mathbf{v}_c = \mathbf{v}_{\ell_2}(BN)^{-1}$, and has a zero entry only if $\mathbf{v}_{\ell_2}$ is in the left nullspace of one (or more) of the columns of $(BN)^{-1}$. However, replacing A and B with AC and $C^{-1}B$ for some appropriate nonsingular matrix C whose rows sum to one, we can ensure that $\mathbf{v}_c$ has no zero entries.

Since the parameters producing Q' are nonsingular, by Lemma 5.2 we may reroot T_1 at c, with parameters the root distribution $\mathbf{v}_c$, matrices $\{M_e\}$ on all edges of T_1 corresponding to ones in T, and matrix $M_{(c,a)}$ on the edge (c, a).

Now with K the matrix which marginalizes $\mathrm{Flat}_{e_0}(P)$ over all elements of L_1 but one, say ℓ_1, we see

$$K\,\mathrm{Flat}_{e_0}(P) = KAB = \mathrm{Flat}_{e_2}(U),$$

where U is the marginalization of P over the same elements of L_1 and the last flattening is on $e_2 = (b, \ell_1)$ in the induced subtree, which is isomorphic to T_2. But by induction U arises from nonsingular parameters on T_2 rooted at b. Letting M be the product of the matrix parameters on the edges in the path from c to ℓ_1 in T_1. Then $U' = U *_{\ell_1} M^{-1}$ also arises from nonsingular parameters on T_2 (checking that its marginalization to c is $\mathbf{v}_{\ell_1} M^{-1} = \mathbf{v}_c$, which has no zeros by construction).

Note now that U' has flattening $(M^{-1})^T KAB$. But $(M^{-1})^T KA = \operatorname{diag}(\mathbf{v}_c)$ by construction. Thus $\operatorname{diag}(\mathbf{v}_c)B$ is the $c|L_2$ flattening of a tensor arising on T_2 from nonsingular complex parameters. With the root at c, let M_e be the Markov parameters for all edges of T_2 corresponding to ones in T, and $M_{(c,b)}$ the Markov matrix on (c, b). The root distribution $\mathbf{v}_c$ is the same as for T_1.

It remains to check that P is the image of the parameters on T with subdivided edges (c, a) and (c, b) rooted at c given by $\mathbf{v}_c$, $\{M_e\}_{e \neq (a,b)}$, and $M_{(c,a)}$ and $M_{(c,b)}$. But these parameters lead to the distributions Q' and U' on T_1 and T_2 respectively. Since $\operatorname{Flat}_{(a,c)}(Q') = A$ while $\operatorname{Flat}_{(c,b)}(U') = \operatorname{diag}(\mathbf{v}_c)B$, the equation $\operatorname{Flat}_e(P) = AB$ shows they produce P on T.

That the parameters are unique, up to label swapping at the internal nodes of T, follows from the 3-leaf case. ∎

Note that in establishing the reverse implication in Proposition 5.5 we did not use condition (i) for every 3-variable marginalization. Informally, given a tree T one could choose a sequence of edges which can be successively 'cut' (by the introduction of the node c in the inductive proof above) to produce a forest of 3-taxon trees. Then condition (i) is only needed for a subset of the 3-leaf marginalizations, determined by the sequence of edges chosen to cut and the choice of the variables denoted ℓ_1, ℓ_2 in the proof. Similarly, not all edge flattenings of condition (ii) are used: For the first edge to be 'cut', one uses the full edge flattening, but after that, only edge flattenings of marginalizations to subsets of variables are needed. Thus the full set of conditions given in this proposition is actually equivalent to a subset of them, though pinning down a precise subset is rather messy and will not be pursued here.

Supposing now that an n-dimensional distribution P arises from nonsingular complex parameters on a binary tree T, we wish to give semialgebraic conditions that are satisfied if, and only if, the parameters are stochastic. By considering only marginalizations to 3 variables and appealing to Proposition 3.6, we can give conditions that hold precisely when the root distribution and products of matrix parameters along any path leading from an interior vertex of T to leaves are stochastic. This immediately yields semialgebraic conditions that the root distribution and matrix parameters on terminal edges are stochastic. However, additional criteria are needed to ensure matrix parameters on interior edges are stochastic. In the 4-leaf case, such criteria are given by the following.

Proposition 5.6. *Suppose a tensor P arises from nonsingular complex parameters for GM(k) on the 4-leaf tree $12|34$. If the 3-marginalizations $P_{\cdot\cdot\cdot+}$ and $P_{+\cdot\cdot\cdot}$ arise from stochastic parameters and, in addition, all principal minors of the $k^2 \times k^2$ matrix*

$$\det(P_{+\cdot\cdot+}) \det(P_{\cdot+\cdot+}) \operatorname{Flat}_{13|24}\left(P *_2 (\operatorname{adj}(P_{+\cdot\cdot+}^T) P_{\cdot+\cdot+}^T)) *_3 (\operatorname{adj}(P_{\cdot+\cdot+}) P_{\cdot++\cdot})\right) \quad (5.1)$$

are nonnegative, then P arises from stochastic parameters.

The statement about the minors of the symmetric matrix in (5.1) is of course really a requirement that this matrix be positive semidefinite. Also, this matrix could instead be replaced by ones where the roles of leaves 1 and 2 or of leaves 3 and 4 have been interchanged.

Proof. Root T at the interior node near leaves 1 and 2. Let M_i, $i = 1, 2, 3, 4$ be the complex matrix parameter with row sums equal to one on the edge leading to leaf

i, M_5 the matrix parameter on the internal edge, and $\boldsymbol{\pi}$ the root distribution. Define the matrices

$$N_{32} = P^T_{+\cdot\cdot+} = M_3^T M_5^T \operatorname{diag}(\boldsymbol{\pi}) M_2,$$
$$N_{31} = P^T_{\cdot+\cdot+} = M_3^T M_5^T \operatorname{diag}(\boldsymbol{\pi}) M_1.$$

Then

$$\overline{P} = P *_2 N_{32}^{-1} N_{31}$$

is a tensor arising from the same parameters as P except that M_2 has been replaced with M_1. That is, now the same matrix parameter is used on the edges leading to leaves 1 and 2.

Similarly with

$$N_{14} = P_{\cdot++\cdot} = M_1^T \operatorname{diag}(\boldsymbol{\pi}) M_5 M_4,$$
$$N_{13} = P_{\cdot+\cdot+} = M_1^T \operatorname{diag}(\boldsymbol{\pi}) M_5 M_3,$$

then

$$\widetilde{P} = \overline{P} *_3 N_{13}^{-1} N_{14} \tag{5.2}$$

is a tensor arising from the same parameters as $\overline{P}$ except that M_3 has been replaced with M_4.

Consider now the $13|24$ flattening of $\widetilde{P}$, a flattening which is *not* consistent with the topology of the underlying tree. As shown in [5], this can be expressed as a product of $k \times k$ matrices

$$\operatorname{Flat}_{13|24}(\widetilde{P}) = A^T D A, \tag{5.3}$$

where D is the diagonal matrix with the k^2 entries of $\operatorname{diag}(\boldsymbol{\pi}) M_5$ on its diagonal, and $A = M_1 \otimes M_4$ is the Kronecker product. Because M_1, M_4 are nonsingular, so is A. Since conditions on 3-marginals ensure $\boldsymbol{\pi}$ has positive entries, we can ensure M_5 has nonnegative entries by requiring that $\operatorname{Flat}_{13|24}(\widetilde{P})$ be positive semidefinite. Using Sylvester's theorem, this is equivalent to requiring that its principal minors be nonnegative. Since the resulting inequalities would involve rational expressions, due to the inverses of matrices, we first multiply $\operatorname{Flat}_{13|24} \widetilde{P}$ by squares of nonzero determinants, to remove denominators. ∎

The matrix in (5.1) has entries of degree $4k+1$ in those of P. After removing squares of powers of determinants for even minors, the polynomial inequalities from the principal $j \times j$ minors are of degrees $j(2k+1) + 2ke_j$, where $e_j \in \{0, 1\}$ gives the parity of j.

Together with Theorems 3.6 and 3.7, the last two propositions yield the following theorem.

THEOREM 5.7. *Suppose P is an n-dimensional joint probability distribution for the k-state variables $Y_1, \dots, Y_n$. Then P arises from nonsingular stochastic parameters for GM(k) on an n-leaf binary tree T if, and only if,*

(i) *All marginalizations of P to 3 variables satisfy the conditions of Theorem 3.6 (or if $k = 2$ of Theorem 3.7) to arise from nonsingular stochastic parameters on a 3-leaf tree;*

(ii) *For all internal edges e of T, the edge invariants are satisfied by P, i.e., all $(k+1)\times(k+1)$ minors of the matrix flattening $Flat_e(P)$ are 0;*

(iii) *For each internal edge e of T, and some choice of 4 leaves inducing a quartet tree with internal edge e, all principal minors of the matrix flattening constructed in Proposition 5.6, for the 4-dimensional marginalization, are nonnegative.*

While we noted that one can use a smaller set of inequalities than were given in Proposition 5.5 to ensure a distribution arises from nonsingular parameters, the full set of inequalities given in Theorem 5.7 has additional redundancies. To illustrate, in the 4-leaf case checking that only two of the 3-marginals, say $P_{+\cdots}$ and $P_{\cdots+}$ for the tree 12|34, satisfy the conditions of Proposition 3.6. is sufficient.

For a 4-variable distribution P, it is straightforward to obtain semialgebraic conditions ensuring P arises from strictly positive parameters: One need only require the more stringent condition (iv') of Proposition 3.6, on the marginalizations $P_{\cdots+}$ and $P_{+\cdots}$ to ensure they arise from strictly positive parameters, and that all leading principal minors of the matrix in (5.1) are strictly positive. This then allows one to give such conditions applicable to larger trees, establishing the following.

Theorem 5.8. *Semialgebraic conditions that a probability distribution P arises from nonsingular positive parameters for* GM(k) *on a tree T can be explicitly given.*

Note that one can also handle non-binary trees by the techniques of this section. To show a distribution arises from nonsingular, or stochastic nonsingular, parameters on a non-binary tree, one need only show it arises from parameters on a binary resolution of the tree, and that the Markov matrix on each edge introduced to obtain the resolution is the identity. But semialgebraic conditions that the Markov matrix on an internal edge of a 4-leaf tree be I (or a permutation, since label swapping prevents us from distinguishing these) amounts to requiring that the matrix of equation (5.3) has rank k. Indeed, rank k implies that the Markov matrix on the internal edge has only k nonzero entries, and since other conditions we have derived imply nonsingularity, the matrix must be a permutation.

We now give an example illustrating that the quadratic form approach of Proposition 5.6, and thus of Theorem 5.7, detects a probability distribution that is in the image of ψ_T for nonsingular real GM(2) parameters on the 4-taxon tree, where each matrix parameter on a terminal edge is stochastic but the one on the internal edge is not. By choosing parameters with some care, we can arrange that such a probability distribution P satisfies that all 3-marginalizations arise from stochastic parameters, yet P does not. Such examples are not new (see for example [4, 23, 37]), but we include one here to illustrate our methods.

To create such an example, set the Markov parameter on each terminal edge to have positive entries, using, for instance, the same M on each of these 4 edges. Then choose the matrix parameter N on the internal edge of the tree to have very small negative off-diagonal entries, so small so that both MN and NM are Markov matrices. The root distribution may be taken to be any probability distribution with positive entries. An example of such an (exact) probability distribution is given by P with slices

$$P_{\cdot\cdot 11} = \begin{bmatrix} 0.4005062 & 0.0565718 \\ 0.0565718 & 0.0545702 \end{bmatrix} \qquad P_{\cdot\cdot 12} = \begin{bmatrix} 0.0457358 & 0.0141662 \\ 0.0141662 & 0.0379118 \end{bmatrix}$$
$$P_{\cdot\cdot 21} = \begin{bmatrix} 0.0457358 & 0.0141662 \\ 0.0141662 & 0.0379118 \end{bmatrix} \qquad P_{\cdot\cdot 22} = \begin{bmatrix} 0.0100222 & 0.0330958 \\ 0.0330958 & 0.1316062 \end{bmatrix}.$$

Here P satisfies all conditions of Theorem 5.7 except (iii). A computation shows that the principal minors of the matrix in (5.1) are, when rounded to eight decimal places, 0.00363408, 0.00001744, 0.00000060, and −0.00000005. The negativity of one of these shows P does not arise from stochastic parameters.

We conclude with a complete semialgebraic description of the 2-state general Markov model on a 4-leaf tree without a restriction to nonsingular stochastic parameters. This is straightforward to give, since Proposition 2.2 indicates that in this case a distribution which arises from parameters either has independent leaf sets (so we can decompose the tree using Proposition 5.3), or the parameters were nonsingular so Theorem 5.7 applies.

As observed earlier, the existence of many non-independence cases when $k > 2$ prevents us from assembling as complete a result.

Proposition 5.9. *For the* 4*-leaf tree* $12|34$*, the image of the stochastic parameter space under the general Markov model* $GM(2)$ *is the union of the following sets of nonnegative tensors whose entries add to 1:*

1. *Probability distributions of* 4 *independent variables:* P *such that all* 2×2 *minors of every edge flattening vanish (i.e., all edge flattenings have rank 1);*
2. *Probability distributions with partition into minimal independent sets of variables of size* 1, 3*, of which there are 4 cases: If the partition is* $\{\{Y_1\}, \{Y_2, Y_3, Y_4\}\}$*, then* P *such that all* 2×2 *minors of* $\mathrm{Flat}_{1|234}(P)$ *vanish, and* $P_{+\cdot\cdot\cdot}$ *satisfies the conditions of Theorem 3.7, Case 1;*
3. *Probability distributions with partition into minimal independent sets of variables of size* 1, 1, 2*, of which there are 6 cases: If the partition is* $\{Y_1\}|\{Y_2\}|\{Y_3, Y_4\}$*, then* P *such that all* 2×2 *minors of* $\mathrm{Flat}_{1|234}(P)$ *and* $\mathrm{Flat}_{2|134}(P)$ *vanish, and* $\det(P_{++\cdot\cdot})$ *is nonzero;*
4. *Probability distributions with partition into minimal independent sets of variables* $\{\{Y_1, Y_2\}, \{Y_3, Y_4\}\}$ *of size* 2, 2*:* P *such that all* 2×2 *minors of* $\mathrm{Flat}_{12|34}(P)$ *vanish, yet* $\det(P_{\cdot\cdot++})$ *and* $\det(P_{++\cdot\cdot})$ *are nonzero,*
5. *Probability distributions with no independent sets of variables:* P *such that the edge invariants for* $12|34$ *are satisfied, the* 3*-d marginalizations* $P_{+\cdot\cdot\cdot}$ *and* $P_{\cdot\cdot\cdot+}$ *satisfy the conditions of Theorem 3.7, Case 1, and all principal minors of the matrix constructed in Proposition 5.6 are nonnegative.*

In case 1, the only edge flattenings that are needed are those associated to terminal edges. If these all have rank 1, then the flattening for the internal edge does as well.

In cases 1,2,3, the distributions arise from stochastic parameters on all 3 of the binary topological trees with 4 leaves, as well as the star tree.

Note that all possible partitions of variables do not appear, but only those consistent with the tree topology. In the 4-leaf case, this has ruled out only the 2 partitions of size 2,2 that do not reflect a split in the tree.

Of course one could extend the above proposition to arbitrary size trees, as long as $k = 2$, but the number of possible partitions into independent sets of variables grows quickly, so we will not give an explicit statement.

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