DISTANCE TO THE STOCHASTIC PART OF PHYLOGENETIC VARIETIES

MARTA CASANELLAS, JESÚS FERNÁNDEZ-SÁNCHEZ, AND MARINA GARROTE-LÓPEZ

Abstract. Modelling the substitution of nucleotides along a phylogenetic tree is usually done by a hidden Markov process. This allows to define a distribution of characters at the leaves of the trees and one might be able to obtain polynomial relationships among the probabilities of different characters. The study of these polynomials and the geometry of the algebraic varieties that define can be used to reconstruct phylogenetic trees. However, not all points in these algebraic varieties have biological sense. In this paper, we explore the extent to which adding semialgebraic conditions arising from the restriction to parameters with statistical meaning can improve existing methods of phylogenetic reconstruction. To this end, our aim is to compute the distance of data points to algebraic varieties and to the stochastic part of these varieties. Computing these distances involves optimization by nonlinear programming algorithms. We use analytical methods to find some of these distances for quartet trees evolving under the Kimura 3-parameter or the Jukes-Cantor models. Numerical algebraic geometry and computational algebra play also a fundamental role in this paper.

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1. Introduction

Within the new century, algebraic tools have started to be successfully applied to some problems of phylogenetic reconstruction (see for example [1, 14, 2]). The main goal of phylogenetic reconstruction is to estimate the phylogenetic tree that best explains the evolution of living species using solely information of their genome. To this end, one usually considers evolutionary models of molecular substitution and assume that DNA sequences evolve according to these models by a Markov process on a tree. Some of the most used models are nucleotide substitution models (e.g. Kimura 3-parameter [24] or Jukes-Cantor [23] models), which are specified by a $4 \times 4$ transition matrix associated to each edge of the tree and a distribution of nucleotides at the root. Then, the distribution of possible nucleotide sequences at the leaves of the tree (representing the living species) can be computed as an algebraic expression in terms of the parameters of the model (the entries of the substitution matrices and the distribution at the root). This allows the use of algebraic tools for phylogenetic reconstruction purposes.

When reconstructing the tree topology (i.e., the shape of the tree taking into account the names of the species at the leaves), the main tools that have been used come either from rank conditions on matrices arising from a certain rearrangement of the distribution of nucleotides at the leaves [13, 14, 19], or from phylogenetic invariants [28, 10]. These tools use the fact that the set of possible distributions satisfies certain algebraic constraints, but do not specifically use the condition that one is dealing with discrete distributions that arise from stochastic matrices at the edges of the tree (i.e. with positive entries and rows summing to one). These extra conditions lead to semi-algebraic constraints which have been specified for certain models in [8] (for the general Markov model), [29] (for the Kimura 3-parameter model) and [33, 25] for the 2-state case ($2 \times 2$ transition matrices). Combining algebraic and semi-algebraic conditions to develop a tool for reconstructing
the tree topology is not an easy task and, as far as we are aware, both tools have only been used together in [26] for the simple case of 2 states.

As a starting point of topology reconstruction problems, it is natural to use trees on four species (called 1,2,3,4 for example). In this case, there are three possible (unrooted and fully resolved) phylogenetic trees, 13|24, 13|24, and 14|23 (see Figure 1). Then a distribution of nucleotides for this set of species is a vector \( P \in \mathbb{R}^4 \) whose entries are non-negative and sum to one. The set of distributions arising from a Markov process on any of these trees \( T \) (for a given substitution model) defines an algebraic variety \( V_T \) (see Section 2.1). The three phylogenetic varieties \( V_{12|34}, V_{13|24}, V_{14|23} \) are different and the topology reconstruction problem for a given distribution \( P \in \mathbb{R}^4 \) is, briefly, deciding to which of these three varieties \( P \) is closest (for a certain distance or for another specified optimization problem such as likelihood estimation). The algebraic tools related to rank conditions mentioned above attempt to estimate these euclidean distances, for example.

If we assume that \( P \) should be close to a distribution that has arisen from stochastic parameters on one of these trees, then one should consider only the stochastic part of these varieties, \( V_{12|34}^+, V_{13|24}^+, V_{14|23}^+ \) (which we call the stochastic phylogenetic varieties). The main questions that motivated the study presented here are:

Could semi-algebraic tools add some insight to the already existent algebraic tools? Do semi-algebraic conditions support the same tree \( T \) whose algebraic variety \( V_T \) is closest to the data point?

In terms of the Euclidean distance and trees of four species, we make the explicit following question:

**Question 1:** If \( P \in \mathbb{R}^4 \) is a distribution satisfying \( d(P, V_{12|34}) < \min\{d(P, V_{13|24}), d(P, V_{14|23})\} \), would it be possible that \( d(P, V_{12|34}^+) > \min\{d(P, V_{13|24}^+), d(P, V_{14|23}^+)\} \)?

We address this problem for special cases of interest in phylogenetics: short branches at the external edges (see section 4) and long branch attraction (in section 6). The length of a branch in a phylogenetic tree is understood as the expected number of substitutions of nucleotides per site along the corresponding edge; both cases, short and long branches, usually lead to confusing results in phylogenetic reconstruction (particularly in relation to the long branch attraction problem, see section 6). In the first case we are able to deal with the Kimura 3-parameter model and in the second case we have to restrict to the more simple Jukes-Cantor (JC69) model. The reason for this restriction is that the computations get more involved in the second case and we have to use computational algebra techniques (for which is crucial to decrease the number of variables of the problem). To this end, in section 5 we introduce an algorithm that computes the distance of a point to the stochastic phylogenetic varieties in the JC69 case; this algorithm makes explicit use of the euclidean distance degree [16] of the phylogenetic varieties.

![Figure 1. The three unrooted (fully resolved) phylogenetic trees on 4 leaves: 12|34 (left), 13|24 (middle) and 14|23 (right)](image-url)
We find that in the first framework (short external branches), restricting to the stochastic part does not make any difference, that is Question 1 has a negative answer in this case (see Theorem 4.3). However, in the long branch attraction framework, considering the stochastic part of phylogenetic varieties might be of interest, specially if the data points are close to the intersection of the three varieties, see Theorem 6.7. In particular, the answer to Question 1 is positive for data close to the long branch attraction problem under the JC69 model. In section 7 we provide results on simulated data that support these findings and also show a positive answer to Question 1 for balanced trees.

Summing up, incorporating the semi-algebraic conditions to the problem of phylogenetic reconstruction seems important when the data are close to the intersection of the three phylogenetic varieties. This is the case where phylogenetic reconstruction methods tend to confuse the trees. On the contrary, on data points which are far from the intersection (in the short branches case of section 4 for example), it does not seem necessary to incorporate these semi-algebraic tools. This is the reason why incorporating these tools into phylogenetic reconstruction methods might be extremely difficult.

The organization of the paper is as follows. In section 2, we introduce the concepts on nucleotide substitution models and phylogenetic varieties that we will use later on. Then in section 3 we prove some technical results regarding the closest stochastic matrix to a given matrix. In section 4 we consider the case of short external branches for the Kimura 3-parameter model and obtain the results analytically. In section 5 we introduce the computational approach that we use in order to compute the distance to the stochastic phylogenetic varieties. The results for the long branch attraction case are expanded in section 6 and in section 7 we provide results on simulated data that illustrate our findings. The Appendix collects all technical proofs needed in section 6.

2. Preliminaries

2.1. Phylogenetic varieties. We refer the reader to the work [6] of E. A. Allman and J. A. Rhodes for a good general overview of phylogenetic algebraic geometry. Here we briefly introduce the basic concepts that will be needed later. Let $T$ be a phylogenetic tree with its leaves labelled by $\{1, 2, 3, 4\}$ (i.e. $T$ is a tree as a graph whose interior nodes have degree 3 and whose leaves, of degree 1, are in correspondence with $\{1, 2, 3, 4\}$), see Figure 1. Using the notation introduced in Figure 1, $T$ belongs to the set $T = \{12|34, 13|24, 14|23\}$. When the tree $T$ needs to be considered as rooted, we will choose an internal vertex $r$ as the root. Suppose the Markovian evolutionary process on that tree follows a nucleotide substitution model $M$: associate a random variable taking values on $\Sigma := \{A, C, G, T\}$ at each node of the tree, and consider as parameters the distribution $\pi = (\pi_A, \pi_C, \pi_G, \pi_T)$ at the root, $\sum_i \pi_i = 1$, and a $4 \times 4$ transition matrix $M_e$ at each edge $e$ of $T$. The transition matrices are stochastic (or Markov) matrices, that is, all its entries are nonnegative and sum up to 1. A vector is stochastic if all its coordinates are nonnegative and sum up to 1.

If $T \in T$ and $S$ is the set of stochastic parameters described above, we denote by $\psi_T$ the following (parametrization) map:

$$\psi_T : S \subset [0, 1]^6 \to \mathbb{R}^{4^4}$$

$$\{\pi, \{M_e\}_{e \in E(T)}\} \mapsto P = (p_{AAAA}, p_{AAAC}, \ldots, p_{TTTG}, p_{TTTT})$$

which maps each set of parameters of the model $\{\pi, \{M_e\}_{e \in E(T)}\} \in S$ to the joint distribution of characters at the leaves of $T$ given by the hidden Markov process on $T$ governed by these parameters. The entries $p_{x_1,\ldots,x_4}$ of the joint distribution can be expressed in
terms of the entries of the substitution matrices. For example, for the tree 12|34 rooted at the leftmost internal edge with transition matrices as in Figure 2 we have

$$p_{x_1, x_2, x_3, x_4} = \sum_{x_r, x_s \in \Sigma} \pi_{x_r} M_1(x_r, x_1) M_2(x_r, x_2) M_5(x_r, x_s) M_3(x_s, x_3) M_4(x_s, x_5)$$

**Figure 2.** Tree 12|34 with transition matrices $M_1, M_2, M_3, M_4$ and $M_5$

We write $V_T^+$ for the image of $\psi_T$, that is, the space of all the distributions arising from stochastic parameters,

$$V_T^+ = \{ P \in V_T \mid P = \psi_T(s) \text{ and } s \in S \}.$$

We call this set the *stochastic phylogenetic variety.*

Since $\psi_T$ is a polynomial map, it can be extended to $\mathbb{R}^\ell$ (that is, we can consider not only nonnegative entries in $\pi$ and $M_e$). Define the *phylogenetic variety* associated with $T$ as the smallest algebraic variety containing $\psi_T(\mathbb{R}^\ell)$,

$$V_T = \overline{\psi_T(\mathbb{R}^\ell)}.$$

This variety contains all joint distributions that arise from the model $M$ on the tree $T$ and some additional points in the closure of that set. Thus, not every point in these varieties has biological sense.

**Remark 2.1.** Unless noted otherwise we will always assume rows of the matrices $M_e$ sum up to 1, even if the entries are not positive (as in the extension of the map $\psi_T$ just defined).

### 2.2. Kimura and Jukes-Cantor models.

In this paper we focus on phylogenetic 4-leaf trees evolving under the *Jukes-Cantor* (JC69 for short, see [23]) and the 3-parameter *Kimura* (K81 for short, [24]) models. The JC69 model is a highly structured model that assumes equal mutation probabilities while the K81 takes into account the classification of nucleotides as purines/pyrimidines and the probabilities of substitution between and within these groups. Both models assume the uniform distribution at the root, $\pi = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$.

**Definition 2.2.** A $4 \times 4$ matrix $M$ is a *K81 matrix* if it is of the form

$$M = \begin{pmatrix}
  a & b & c & d \\
  b & a & d & c \\
  c & d & a & b \\
  d & c & b & a
\end{pmatrix},$$

for some $a, b, c, d \in \mathbb{R}$ summing to 1, $a + b + c + d = 1$. If $b = c = d$, then we say that $M$ is a *JC69 matrix.*
Note that these matrices only have an interpretation as transition matrices of a Markov process if they only have nonnegative entries; in this case we talk about stochastic K81 matrices or stochastic JC69 matrices.

**Lemma 2.3.** ([1]) If $M$ is a K81 matrix as $[1]$, then it diagonalizes with eigenvalues $m_A = a + b + c + d = 1$, $m_C = a + b - c - d$, $m_G = a - b + c - d$ and $m_T = a - b - c + d$ and respective eigenvectors $\bar{A} = (1, 1, 1, 1)^t$, $\bar{C} = (1, 1, -1, -1)^t$, $\bar{G} = (1, -1, 1, -1)^t$ and $\bar{T} = (1, -1, -1, 1)^t$. In particular, the eigenvalues of a JC69 matrix are $m_A = 1$ and $m_C = m_G = m_T = 1 - 4b$.

### 2.3. Fourier coordinates

Let $M$ be a K81 matrix and write $m_A, m_C, m_G, m_T$ and $\bar{A}, \bar{C}, \bar{G}, \bar{T}$ for the eigenvalues and eigenvectors of $M$, respectively. The basis of eigenvectors will be denoted by $\bar{\Sigma} = \{\bar{A}, \bar{C}, \bar{G}, \bar{T}\}$ and is called the Fourier basis. Because of Lemma 2.3 we have

$$\bar{M} = H^{-1} \cdot M \cdot H,$$

where $\bar{M} = \text{diag}(m_A, m_C, m_G, m_T)$ and

$$H = \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1
\end{pmatrix}$$

is the matrix of change of basis from $\bar{\Sigma}$ to $\Sigma$. Notice that $H^{-1} = \frac{1}{4} H^t = \frac{1}{4} H$.

The vectors $P = (p_{AAAA}, p_{AAAC}, \ldots, p_{TTTT}, \bar{p}_{TTTT}) \in \mathbb{R}^4$ considered in section 2.1 can be thought of as $4 \times 4 \times 4 \times 4$ tensor in $\otimes^4 \mathbb{R}^4$: if we call $\Sigma = \{A, C, G, T\}$ the standard basis of $\mathbb{R}^4$, then the components $p_{x_1 x_2 x_3 x_4}$ of $P$ is its coordinates in the natural basis in $\otimes^4 \mathbb{R}^4$ induced by $\Sigma$. This motivates the following definition.

**Definition 2.4.** Given a tensor $P$ in $\mathbb{R}^4 \otimes \mathbb{R}^4 \otimes \mathbb{R}^4 \otimes \mathbb{R}^4$, we will denote by $(p_{AAAA}, p_{AAAC}, \ldots, p_{TTTT})^t$ the coordinates of $P$ in the basis $\{A \otimes A \otimes A \otimes A, A \otimes A \otimes A \otimes C, \ldots, T \otimes T \otimes T \otimes T\}$ induced by $\Sigma$. Similarly, we will write $(\bar{p}_{AAAA}, \bar{p}_{AAAC}, \ldots, \bar{p}_{TTTT}, \bar{p}_{TTTT})^t$ for the coordinates of $P$ in the basis $\{\bar{A} \otimes \bar{A} \otimes \bar{A} \otimes \bar{A}, \ldots, \bar{T} \otimes \bar{T} \otimes \bar{T} \otimes \bar{T}\}$ induced by the Fourier basis $\bar{\Sigma}$.

**Remark 2.5.** Note that the Fourier basis is orthogonal and all the vectors have the same norm. Thus, the Euclidean distance between tensors can be computed using the Fourier coordinates (up to a positive scalar).

If one considers the following bijection between $\Sigma$ and the group $G = (\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}, +)$,

$$\Sigma = \{A, C, G, T\} \leftrightarrow \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$$

$A \mapsto (0, 0)$,

$C \mapsto (0, 1)$,

$G \mapsto (1, 0)$,

$T \mapsto (1, 1)$

then the previous change of coordinates can be understood as the discrete Fourier transform on $G^4$. The following result states that the polynomial parametrization $\psi_T$ becomes monomial after this change of coordinates.

**Theorem 2.6.** ([18]) Let $P = \psi_T(\pi, M_1, M_2, M_3, M_4, M_5)$ where $T$ is the tree topology 12|34 and $M_i$ are K81 matrices. If $(m_{A}^i, m_{C}^i, m_{G}^i, m_{T}^i)$ are the eigenvalues of $M_i$, then the
Fourier coordinates of \( P \) are
\[
\bar{p}_{x_1,x_2,x_3,x_4} = \begin{cases} 
\frac{1}{4^4}m_1^1m_2^2m_3^3m_4^4 & \text{if } x_1 + x_2 = x_3 + x_4, \\
0 & \text{otherwise},
\end{cases}
\]
where the sum of elements in \( \Sigma \) is given by the bijection \( \Sigma \leftrightarrow \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z} \) introduced above.

3. The closest stochastic matrix

Throughout this section, we will use the following notation. We write \( H^{n-1} \) for the hyperplane \( \{x_1 + \ldots + x_n = 1\} \). Given a point \( v \in \mathbb{R}^n \), we denote by \( \text{proj}_H(v) \) and \( \text{proj}_\triangle(v) \) the orthogonal projections of \( v \) onto \( H^{n-1} \) and the standard \((n-1)\)-dimensional simplex \( \triangle^{n-1} \), respectively.

Definition 3.1. For any matrix \( M \in \mathcal{M}_n(\mathbb{R}) \) we denote by \( \hat{M} \) its closest matrix in the Frobenious norm:
\[
\hat{M} = \arg \min_X \| M - X \|_F.
\]

Similarly, for any vector \( v \) we write \( \hat{v} \) for its closest stochastic vector.

The problem of finding the nearest stochastic matrix is equivalent to finding the orthogonal projection (in Euclidean norm) of every row of the matrix onto the standard simplex \( \triangle^{n-1} \). The uniqueness of \( \hat{v} \), and consequently of \( \hat{M} \), is guaranteed since both the objective function and the domain set are convex. The orthogonal projection onto the standard simplex has been widely studied and there exist several algorithms to compute it. We refer the reader to [30] for an algorithm that, given any vector \( v \in \mathbb{R}^n \), produces a vector \( x \in \mathbb{R}^n \) with \( \sum_i x_i = 1 \) and \( x_i \geq 0 \) that minimizes \( \| v - x \|_2 \).

In the following result we state some properties of this last projection that will be useful later.

Lemma 3.2. Let \( v = (v_1, \ldots, v_n) \) be a point in \( \mathbb{R}^n \) and let \( \hat{v} = (\hat{v}_1, \ldots, \hat{v}_n) \) be its orthogonal projection onto \( \triangle^{n-1} \), \( \hat{v} := \text{proj}_\triangle(v) \).

(i) \( \text{proj}_\triangle(v) = \text{proj}_\triangle \left( \text{proj}_H(v) \right) \)
(ii) If \( v \in H^{n-1} \) and \( v_i \leq 0 \) for some \( i \), then \( \hat{v}_i = 0 \).
(iii) Let \( w \) be a point obtained by a permutation of the coordinates of \( v \), i.e. \( w = P v \) for some permutation matrix \( P \). Then \( \hat{w} = P \hat{v} \).
(iv) If \( v_i = v_j \) for some \( i, j = 1, \ldots, n \) then \( \hat{v}_i = \hat{v}_j \).
(v) The projection of \( v \) is \( p_i = (0, \ldots, 1 \atop i, \ldots, 0) \) if and only if \( v_i - v_j \geq 1 \ \forall j \neq i \).

Proof. The proofs of items (i) and (ii) can be found in [30]. These two statements also suggest a method to compute the projection onto the standard simplex.

(iii) This follows from the fact that \( P \) is a permutation matrix and hence is an orthogonal matrix.

(iv) It is a consequence of (iii).
Using (i) and (ii) we can assume that $\sum_i v_i = 1$, i.e., $v$ belongs to the affine hyperplane $H^{n-1}$.

We will use $p_i$ to denote the vertex $(0, \ldots, 1, \ldots, 0)$ of $\Delta^{n-1}$, $F_i$ to denote the facet containing every vertex but $p_i$. We write $w_i$ for the normal vector to $F_i$ contained in $H^{n-1}$.

A parametric expression for the linear subspace of dimension $n-2$ containing the facet $F_i$ is

$$p_j + \sum_{k \neq i} \lambda_k \overrightarrow{p_j p_k} = p_j + \sum_{k \neq i} \lambda_k (0, \ldots, 1, \ldots, 0, \ldots, 1, \ldots, 0)$$

for any $j \neq i$.

The normal vector $w_i$ satisfies $w_i \perp \overrightarrow{p_j p_k}$ and $w_i \perp (1, \ldots, 1)$. An easy computation shows that we can take $w_i := (1, \ldots, 1) - n \cdot \overrightarrow{i}$. Points that are projected onto a vertex $p_i$ of the simplex coincide with the points in a polyhedral convex cone $C_i$ with vertex $p_i$ and rays generated by normal vectors to the facets adjacent to it.

In order to simplify notation, we choose $i = 1$, but the other cases are analogous. The facets adjacent to $p_1 = (1, 0, \ldots, 0)$ are $F_2, \ldots, F_n$. The 2-dimensional faces of the cone $C_1$ are generated by $p_1$ and the subspace generated by any two vectors of $w_2, \ldots, w_n$.

For instance the parametric expression of the face generated by $w_2$ and $w_3$ is

$$H_{2,3}^{n-1} = p_1 + \lambda_2 w_2 + \lambda_3 w_3 = (1, 0, \ldots, 0) + \lambda_2 (1, 1-n, 1, \ldots, 1) + \lambda_3 (1, 1, 1-n, \ldots, 1)$$

$$= (1 + \lambda_2 + \lambda_3, (1-n)\lambda_2 + \lambda_3, \lambda_2 + (1-n)\lambda_3, \lambda_2 + \lambda_3, \ldots, \lambda_2 + \lambda_3)$$

with $\lambda_2 \geq 0$ and $\lambda_3 \geq 0$. After some computations, one can see that these points can be characterized by the inequalities:

$$x_1 - x_i \geq 1 \quad i = 4, 5, \ldots, n.$$  

If we repeat this computation for every pair of faces we conclude that the points that are projected to $p_1$ are precisely the ones satisfying

$$x_1 - x_j \geq 1 \quad j = 2, 3, \ldots, n.$$  

as we wanted to prove.

\[\square\]

**Remark 3.3.** If the rows of a matrix $M$ result of some permutation applied to the first row, the previous lemma shows that $\hat{M}$ will preserve the same identitites between entries as the matrix $M$. Actually, it can be shown that if $M$ is a matrix in a equivariant model [17] not necessarily stochastic, then $\hat{M}$ will remain in the same model.

The following lemma is direct and the proof is left to the reader.

**Lemma 3.4.** Let $M$ be a $JC69$ matrix. Then $M$ is stochastic if and only if its eigenvalues are contained in $[-1/3, 1]$.

**Lemma 3.5.** Let $M$ be a non-stochastic Jukes-Cantor matrix. Then $\hat{M}$ is either the identity matrix or the matrix

$$
\begin{pmatrix}
0 & 1/3 & 1/3 & 1/3 \\
1/3 & 0 & 1/3 & 1/3 \\
1/3 & 1/3 & 0 & 1/3 \\
1/3 & 1/3 & 1/3 & 0
\end{pmatrix}.
$$
Proof. Let \( M \) be a JC69 with diagonal entries equal to \( a \) and off-diagonal entries equal to \( b \). Then it is not stochastic if either \( b < 0 \) or \( a < 0 \). Let \( v = (a, b, b, b) \) be the first row of \( M \) and \( \hat{v} = (\hat{a}, \hat{b}, \hat{b}, \hat{b}) \) its projection onto the simplex \( \triangle^3 \) (Lemma 3.2 (iv)). The following reasoning is valid for each row because of Lemma 3.2 (iii).

If \( b < 0 \) then, by Lemma 3.2, \( \hat{b} \) equals zero and \( \hat{a} \) has to be equal to 1 since the coordinates of \( \hat{v} \) sum to 1. Therefore \( \hat{M} \) is the \( 4 \times 4 \) identity matrix.

If \( a < 0 \) then \( \hat{a} = 0 \) and since \( 3\hat{b} = 1 \), \( \hat{b} = \frac{1}{3} \). Therefore \( \hat{M} \) is a matrix with 0 in the diagonal and \( \frac{1}{3} \) at the non-diagonal entries. \( \square \)

For later use, we close this section by stating a characterization of those K81 matrices \( M \) for which \( \hat{M} \) is a permutation matrix.

**Lemma 3.6.** Let \( M \) be a K81 matrix and denote by \((a_1, a_2, a_3, a_4)\) its first row. Then \( \hat{M} \) is a permutation matrix if and only if there is some \( i \in \{1, \ldots, 4\} \) such that \( a_i - a_j \geq 1 \) for all \( j \neq i \).

Proof. It is a consequence of Lemma 3.2 (v). \( \square \)

4. Short external branches

In this section we will study evolutionary processes where mutations at the external edges are unusual, so the probabilities of substitution of nucleotides in the corresponding transition matrices are small.

Given \( P \in \mathbb{R}^{4^n} \), let \( P_T^+ \) be a point in \( V_T^+ \) that minimizes the distance to \( P \), i.e.

\[
d(P, P_T^+) = d(P, V_T^+).
\]

Unless noted otherwise we will keep this notation.

**Proposition 4.1.** Assume that \( P = \psi_T(Id, Id, Id, Id, M_e) \) where \( M_e \) is a non-stochastic K81 matrix and \( T \) is any 4-leaf tree. Then,

(a) The point \( P_T^+ \) is equal to \( \psi_T(Id, Id, Id, Id, \hat{M}_e) \). Moreover, it is the point that minimizes the distance to the standard simplex \( \Delta \subset \mathbb{R}^{4^4} \). In particular, the point \( P_T^+ \) is unique.

(b) If \( T' \neq T \) is another tree in \( \mathcal{T} \), then \( d(P, V_{T'}^+) \geq d(P, V_T^+) \).

(c) The following are equivalent:

(i) equality holds in (b);
(ii) \( P_T^+ \in V_T^+ \cap V_{T'}^+ \);
(iii) the matrix \( M_e \) is a permutation matrix.

Proof. We assume that \( T = T_{1234} \), but the proof is analogous for the other trees. We define \( \hat{P} := \text{proj}_\Delta(P) \), that is, \( \hat{P} \) is the only point in \( \Delta \) that minimizes the distance from \( P \) to the standard simplex, which is a convex set. First of all, we have that

\[
d(P, V_T^+) = \min_{Q \in V_T^+} d(P, Q) \geq \min_{Q \in \Delta^{4^4-1}} d(P, Q) = d(P, \hat{P}).
\]

This follows from the fact that \( V_T^+ \subset \Delta^{4^4-1} \), since for all \( Q \in V_T^+ \) the sum of its coordinates \( \sum_i Q_i \) equals 1.
We now show that $\tilde{P} \in \mathcal{V}_T^\perp$. Since the transition matrices at the exterior edges of $T$ are the identity, the coordinates of $P$ are

$$p_{ijkl} = \begin{cases} 
\frac{1}{4}(M_e)_{ik} & \text{if } i = j \text{ and } k = l \\
0 & \text{otherwise.}
\end{cases}$$

Since $M_e$ is a K81 matrix the non-zero coordinates of $P$ only take 4 different values. Moreover, because of Lemma 3.2 (ii) and (iii), we can write the coordinates of $\tilde{P}$ as

$$\tilde{p}_{ijkl} = \begin{cases} 
b_{ik} & \text{if } i = j \text{ and } k = l \\
0 & \text{otherwise.}
\end{cases}$$

for some values $b_{ik}$ satisfying the identities of a K81 matrix. Since $\sum_{i,j} b_{ik} = 1$, it follows that the matrix

$$M = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\
b_{21} & b_{22} & b_{23} & b_{24} \\
b_{31} & b_{32} & b_{33} & b_{34} \\
b_{41} & b_{42} & b_{43} & b_{44} \end{pmatrix}$$

is a K81 stochastic matrix. Actually, this matrix is just $M_e$. In particular, $\tilde{P} \in \mathcal{V}_T^\perp$. Since $P_T^+$ minimizes the distance from $P$ to the variety $\mathcal{V}_T^+$, we have $d(P, \tilde{P}) \geq d(P, P_T^+)$. Because of (2), the equality holds. Moreover, from the uniqueness of the point minimizing the distance to $\Delta$, it follows that $P_T^+ = \tilde{P}$. This concludes the proof of (a).

(b) For any tree topology $T'$, we have that $\mathcal{V}_{T'}^\perp \subset \Delta$. It follows that $d(P, \tilde{P}) \leq d(P, P_{T'}^+)$. Since $\tilde{P} = P_T^+$, we infer that $d(P, P_T^+) \leq d(P, P_{T'}^+)$ for any $T' \neq T$.

Now, we proceed to characterize when the equality holds in (b), which proves (c). (i) $\Leftrightarrow$ (ii). It is clear that if $P_T^+ \in \mathcal{V}_{T'}^\perp$, then $d(P, \mathcal{V}_{T'}^\perp) = d(P, P_{T'}^+) \geq d(P, \mathcal{V}_T^+)$. Together with the inequality in (b), this proves that (ii) implies (i). Conversely, if the equality holds, then $d(P, P_{T'}^+) = d(P, \Delta)$. Because of the uniqueness of the point that minimizes the distance to $\Delta$, it follows that $P_{T'}^+ = \tilde{P}$, and we have already seen that $\tilde{P} \in \mathcal{V}_{T'}^\perp$. Therefore, $P_{T'}^+ \in \mathcal{V}_T^\perp \cap \mathcal{V}_{T'}^\perp$.

(ii) $\Leftrightarrow$ (iii). It only remains to see that $P_T^+ = P_{T'}^+$ (i.e. $P_T^+ \in \mathcal{V}_T^\perp \cap \mathcal{V}_{T'}^\perp$) if and only if $M_e$ is a permutation matrix. If $\tilde{P} \in \mathcal{V}_T^\perp$, then the rank of $\text{flatten}(\tilde{P})$ is less or equal than 4 (see 3). Because $\tilde{P} = \psi_T(Id, \ldots, Id, \hat{M_e})$, $\text{flatten}(P)$ is a diagonal matrix that contains the 16 entries of $\hat{M_e}$ multiplied by a constant (see 7). Since $M_e$ is a K81 stochastic matrix, $\hat{M_e}$ has to be a permutation matrix. Conversely, if $\hat{M_e}$ has to be a permutation matrix, then the corresponding point $\tilde{P} = \psi_T(Id, \ldots, Id, \hat{M_e})$ lies in every variety $\mathcal{V}_T^\perp$.

**Remark 4.2.** Note that $P_T^+$ coincides with $\psi_T(Id, Id, Id, Id, \hat{M_e})$ but also with any tensor obtained by a label swapping of the parameters [5].

**Theorem 4.3.** Let $M$ be a K81 non-stochastic matrix such that $\hat{M}$ is not a permutation matrix (see Lemma 3.6 for a characterization). Let $P_0 = \psi_T(Id, Id, Id, Id, M)$, $T' \neq T$ and let $P \in \mathbb{R}^{4^s}$ be a point such that

$$d(P, P_0) < \frac{d(P_0, \mathcal{V}_T^\perp) - d(P_0, \mathcal{V}_{T'}^\perp)}{2}$$

(this is satisfied if $P$ is close enough to $P_0$). Then $d(P, \mathcal{V}_T^\perp) < d(P, \mathcal{V}_{T'}^\perp)$. 

Proof. We first define the function \( f(Q) = d(Q, V^+_T) - d(Q, V^+_T) \). By hypothesis, \( \hat{M}_c \) is not a permutation matrix and by Proposition 4.1 we have that \( f(P_0) > 0 \). We want to show that \( f(P) > 0 \) if \( d(P, P_0) < f(P_0)/2 \). Clearly, we are done if \( f(P) \geq f(P_0) \), so we assume that \( f(P) < f(P_0) \). From the triangle inequality we have \( |d(P, W) - d(P_0, W)| \leq d(P, P_0) \), for any variety \( W \). Then, we obtain

\[
|f(P) - f(P_0)| = |d(P, V^+_T) - d(P_0, V^+_T) - (d(P, V^+_T) - d(P_0, V^+_T))| \\
\leq |d(P, V^+_T) - d(P_0, V^+_T)| + |d(P, V^+_T) - d(P_0, V^+_T)| \\
\leq 2d(P, P_0) < f(P_0).
\]

Therefore, \( f(P) = (f(P) - f(P_0)) + f(P_0) = -|f(P) - f(P_0)| + f(P_0) > 0 \). This concludes the proof.

Example 4.4. The matrix

\[
M_c = \begin{pmatrix}
0.9 & 0.03 & -0.01 & 0.08 \\
0.03 & 0.9 & 0.08 & -0.01 \\
-0.01 & 0.08 & 0.9 & 0.03 \\
0.08 & -0.01 & 0.03 & 0.9
\end{pmatrix}
\]

satisfies the hypothesis of Theorem 4.3 and its nearest stochastic matrix is

\[
\hat{M}_c = \begin{pmatrix}
0.896 & 0.026 & 0 & 0.076 \\
0.026 & 0.896 & 0.076 & 0 \\
0 & 0.076 & 0.896 & 0.026 \\
0.076 & 0 & 0.026 & 0.896
\end{pmatrix}.
\]

5. Algorithm

Although in the last section we were able to answer our questions analytically, this approach seems unfeasible when we want to tackle more general problems. In this section, in order to find the distance from a point to a stochastic phylogenetic variety we use numerical algebraic geometry. Our goal is to find all critical points of the distance function to a phylogenetic variety in the interior and at the boundary of the stochastic variety. Among the set of critical points we pick the one that minimizes the distance. Similar approaches, where computational and numerical algebraic geometry are applied to phylogenetics studies, can be found in the works [21] and [26].

Let \( \delta_\mathcal{X}(x) \) denote the Euclidean distance of a point \( x \) to an algebraic variety \( \mathcal{X} \),

\[
\delta_\mathcal{X}(x) := d(x, \mathcal{X}).
\]

If \( \mathcal{X}_{\text{sing}} \) is the singular locus of \( \mathcal{X} \), the number of critical points of \( \delta_\mathcal{X}(x) \) in \( \mathcal{X} \setminus \mathcal{X}_{\text{sing}} \) for a general \( x \) is called the Euclidean distance degree (EDdegree for short) of the variety. The EDdegree was introduced in [16] and it is currently an active field of research. According to Lemma 2.1 of [16] the number of critical points of \( \delta_\mathcal{X}(x) \) in \( \mathcal{X} \setminus \mathcal{X}_{\text{sing}} \) is finite and constant for general points \( x \).

In this section we assume the JC69 model and we parametrize each transition matrix by its eigenvalue different from 1 (see Lemma 2.3). From now on, denote by \( P = \varphi_T(x_1, \ldots, x_5) \) the parameterization in the Fourier coordinates, where \( x_i \) is the eigenvalue of the transition matrix \( M_c \). We do not include the root distribution in this notation since for the K81 case it is always the uniform distribution. Recall that by Lemma 3.4 \( P \in V^+_T \) if and only if \( x_i \in [-1/3, 1] \), \( i = 1, \ldots, 5 \).
Given a point \( P \), we denote by \( f_T(x_1, \ldots, x_5) \) the square of the Euclidean distance function from the point \( \varphi_T(x_1, \ldots, x_5) \) to \( P \):

\[
f_T(x_1, \ldots, x_5) = d(P, \varphi_T(x_1, \ldots, x_5))^2,
\]

and by

\[
D := [-1/3, 1]^5
\]

the region of stochastic parameters.

Under the Jukes-Cantor model, the singular points of the varieties \( V_T \) are those that are the image of some null parameter. In other words, \( \varphi_T(x_1, \ldots, x_5) \) is a singular point of the variety if and only if \( x_i = 0 \) for some \( i \) (see [11] and [12] for details).

Hence, we can compute the number of critical points of our function \( f_T \) in the pre-image of the smooth part of the variety as the degree of saturation ideal \( I : (x_1 \cdots x_5)\infty \), where \( I \) is generated by the partial derivatives of \( f_T \). Using this and the package \texttt{Magma} [9] we obtain:

**Lemma 5.1.** If \( V_T \) is the phylogenetic variety corresponding to a 4-leaf tree evolving under the JC69 model, then the EDdegree of \( V_T \) is 290.

For identifying the critical points of this constrained problem we use the \textit{KKT conditions} of first order for local minimums.

**Karush-Kuhn-Tucker conditions (KKT).** If \( f, g_i : \mathbb{R}^l \rightarrow \mathbb{R} \) are \( C^\infty \) functions for \( i = 1, \ldots, n \), we consider the following minimization problem:

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad g_i(x) \leq 0, \ i = 1, \ldots, n.
\end{align*}
\]

If a point \( x^* \) that satisfies \( g_i(x^*) \leq 0 \ \forall \ i = 1, \ldots, m \) is a local optimum of the problem, then there exist some constants \( \mu = (\mu_1, \ldots, \mu_n) \) (called \textit{KKT multipliers}) such that \( x^* \) and \( \mu \) satisfy

(i) \( -\nabla f(x^*) = \sum_{i=1}^n \mu_i \nabla g_i(x^*) \),

(ii) \( \mu_i \geq 0 \ \forall \ i = 1, \ldots, n \),

(iii) \( \mu_i g_i(x^*) = 0 \ \forall \ i = 1, \ldots, n \).

According to these conditions the algorithm falls naturally into two parts. First of all we find the 290 critical points of the objective function over all \( \mathbb{C}^5 \) and then we check the boundary of \( D \).

To find the critical points at the boundary we restrict the function \( f_T \) to all possible boundary subsets and find critical points there. Namely, on the Jukes Cantor model we write

\[
g_{1,i}(x) := x_i - 1 \leq 0 \quad g_{2,i}(x) := -x_i - 1/3 \leq 0
\]

for the inequalities defining the feasible region \( D \). Moreover, for each \( i = 1, \ldots, 5 \) and \( l = 1, 2 \), write

\[
S_{i,l} = \{ x = (x_1, \ldots, x_5) \mid g_{l,i} = 0 \}.
\]

Then \( x \) is at the boundary of \( D \) if it belongs to the subset \( S := (\cap_{i \in \iota_1} S_{1,i}) \cap (\cap_{j \in \iota_2} S_{2,j}) \) for some \( \iota_1, \iota_2 \subseteq \{1, \ldots, 5\} \) disjoint subsets.

We use homotopy continuation methods to solve the different polynomial systems previously described. All computations have been done with the package \texttt{PHCpack.m2} [32] and [22] which turned out to be the only numerical package capable to find these 290 points of \( I : (x_1 \cdots x_5)\infty \). \texttt{Macaulay2} [20] has been used to implement the main core...
of the algorithm while some previous computations have been previously performed with Magma \cite{9}. The whole code can be found in:

(3) \url{https://github.com/marinagarrote/StochasticPhylogeneticVarieties}

\begin{algorithm} 
\textbf{Algorithm 1:} The closest point to a stochastic phylogenetic variety \\
\textbf{Input:} Parameters \(m_1, m_2, m_3, m_4, m_5\) and a topology \(T\).
Compute \(f_T(x)\);
Compute \(I := \left( \frac{\partial f_T}{\partial x_1}, \frac{\partial f_T}{\partial x_2}, \frac{\partial f_T}{\partial x_3}, \frac{\partial f_T}{\partial x_4}, \frac{\partial f_T}{\partial x_5} \right)\);
\(\mathcal{L} := \{\}\); \hfill \text{// Empty list of valid critical points}
d := degree \(I : (x_1 \cdots x_5)^\infty\);
Find the \(d\) 0-dimensional solutions of \(\nabla f_T = 0\);
foreach solution \(x\) do
\quad if \(x \in \mathbb{R}^5\) and \(g_{l, i}(x) \leq 0 \forall l, i\) then
\quad \quad Add \(x\) to \(\mathcal{L}\);
foreach disjoint subsets \(\iota_1, \iota_2 \subseteq \{1, \ldots, 5\}\) do
\quad \quad \(S := (\bigcap_{i \in \iota_1} S_{1, i}) \cap (\bigcap_{j \in \iota_2} S_{2, j})\);
\quad \quad Find the solutions of \(\nabla (f_T)_{|S} = 0\);
\quad \quad if \(x \in \mathbb{R}^5\) and \(g_{l, i}(x) \leq 0 \forall l, i\) then
\quad \quad \quad Add \(x\) to \(\mathcal{L}\);
Evaluate each \(x \in \mathcal{L}\) into \(f_T(x)\) and return the point \(x^*\) with minimum \(f_T(x^*)\);
\textbf{Output:} Parameters \(x_1^*, x_2^*, x_3^*, x_4^*, x_5^*\) such that \(P_T^+ := \varphi_T(x_1^*, \ldots, x_5^*) \in V_T^+\) and \(d(\varphi_T(m_1, \ldots, m_5), V_T^+) = d(\varphi_T(m_1, \ldots, m_5), P_T^+)\)
\end{algorithm}

6. Long branch attraction

\textit{Long branch attraction} is one the most difficult problems to cope with phylogenetic inference. It is a phenomenon in phylogenetic reconstruction when fast evolving lineages are wrongly inferred to be closely related, without considering their true evolutionary relationships. It can happen when a set of similar species contains some that are very different from the main set. Many reconstruction methods join together these outgroup species even though they are very different to each other. Quartet trees representing these events are characterized for having two non-sister long branches and two non-sister short branches.

The length of a branch in a phylogenetic tree represents the expected number of elapsed mutations along that process and, for the K81 and JC69 models, be computed as \(-\log(\det(M))/4\), where \(M\) is the transition matrix associated to the edge. Therefore the branch length of an edge is related to the eigenvalues of the corresponding transition matrix. In particular, for the JC69 model, the eigenvalue different than 1 determines the branch length.

Throughout this section we use the notation introduced in Section 5. Consider the tree of Figure 3 with a non-stochastic matrix \(M_e\) at the interior edge, a stochastic transition matrix \(M\) at edges pointing to leaves 1 and 3, and the identity matrix at the remaining edges. Assume \(M\) and \(M_e\) are Jukes-Cantor matrices. Then, let \(k\) (respectively \(m\)) be the eigenvalue of \(M\) (resp. of \(M_e\)) different from 1. Since \(M\) is stochastic, \(k\) is in \([-1/3, 1]\) (see Lemma 3.4). We also assume \(m > 1\) since \(M_e\) is not stochastic (the
other possibility would be that $m < -1/3$, but this leads to a biologically unrealistic situation. Let $P := \varphi_{12|34}(k,1,k,1,m)$ be the Fourier coordinates of the corresponding joint distribution.

In this section we study the distance of $P$ to the stochastic phylogenetic varieties $V_{12|34}^+, V_{13|24}^+, V_{14|23}^+$ to give an answer to Question 1. As observed in Remark 2.5 we can use Fourier coordinates to compute distances. Given $P = \varphi_{12|34}(k,1,k,1,m)$ and $T \in \mathcal{T}$, we want to find its closest point in $V_T^+$, so our goal is to find $(x_1,\ldots,x_5) \in \mathcal{D}$ such that $d(P, V_T^+) = d(P, \varphi_T(x_1,x_2,x_3,x_4,x_5))$.

![Phylogenetic tree](image)

**Figure 3.** Phylogenetic tree such that $P = \varphi_{12|34}(k,1,k,1,m)$

Therefore, using the notation of Section 5, finding the closest point to $P$ on the stochastic phylogenetic variety $V_T^+$ can be translated into the following optimization problem:

**Problem 6.1.**

\[
\begin{align*}
\text{minimize} & \quad f_T(x) := d(P, \varphi_T(x_1,x_2,x_3,x_4,x_5))^2 \\
\text{subject to} & \quad g_{1,i}(x) \leq 0, \ i = 1,\ldots,5, \\
& \quad g_{2,i}(x) \leq 0, \ i = 1,\ldots,5.
\end{align*}
\]

where $g_{1,i}(x) = x_i - 1$ and $g_{2,i}(x) = -x_i - \frac{1}{3}$.

6.1. **Local minimum.** An initial numerical approach suggests a candidate $x^*$ to be a minimum of this optimization problem when $T = 12|34$. In Fourier coordinates, the Euclidean distance from $P$ to a point $\varphi_{12|34}(x_1,x_2,x_3,x_4,x_5) \in V_{12|34}$ is given by the square root of the following function:

\[
\begin{align*}
&f_{12|34}(x_1,x_2,x_3,x_4,x_5) := 12 \left( x_1 x_2 x_3 x_4 x_5 - k^2 m \right)^2 + 9 \left( x_1 x_2 x_3 x_4 - k^2 \right)^2 + 6 \left( x_1 x_2 x_3 x_5 - k^2 m \right)^2 \\
&\quad + 6 \left( x_1 x_2 x_3 x_5 - km \right)^2 + 6 \left( x_1 x_3 x_4 x_5 - k^2 m \right)^2 + 6 \left( x_2 x_3 x_4 x_5 - km \right)^2 \\
&\quad + 3 \left( x_1 x_3 x_5 - k^2 m \right)^2 + 3 \left( x_2 x_3 x_5 - km \right)^2 + 3 \left( x_1 x_4 x_5 - km \right)^2 \\
&\quad + 3 \left( x_2 x_4 x_5 - m \right)^2 + 3 \left( x_1 x_2 - k \right)^2 + 3 \left( x_3 x_4 - k \right)^2.
\end{align*}
\]

We define $x^* = (\kappa(k,m),1,\kappa(k,m),1,1)$ where $\kappa(k,m)$ is the minimum between 1 and the unique real solution $\bar{x}(k,m)$ of $\frac{\partial f_{12|34}}{\partial x_1}(x_1,1,x_1,1,1) = 0$. A direct computation shows that,
minimum of the optimization problem 6.1 for

\[ T \]

conditions, we need to take the minimum of the optimization problem 6.1 where \( T \) is either 12 or 13.

Moreover, \( x^* \) is a local minimum we first show that \( x^* \) satisfies the Karush-Kuhn-Tucker (KKT) conditions defined in Section 5 for some KKT multipliers \( \mu_{i,1}, \mu_{2,i}, i = 1, \ldots, 5 \).

Assume first that \( x^* \) is a local minimum we first show that \( x^* \) satisfies the Karush-Kuhn-Tucker (KKT) conditions defined in Section 5 for some KKT multipliers \( \mu_{i,1}, \mu_{2,i}, i = 1, \ldots, 5 \).

Theorem 6.4. If \( k \in [-1/3, 1) \) and \( m \in \Omega := (1, \omega] \), where \( \omega = \frac{4}{9} + \frac{11}{27} \sqrt{69 + 16\sqrt{3}} + \sqrt{\frac{69 + 16\sqrt{3}}{243}} \approx 1.734 \),

Remark 6.3. For \( m > \omega \) there exists some values of \( k \in [-1/3, 1) \) where \( x^* \) is still well defined. Nevertheless, in the phylogenetic framework we are working, it is enough to consider the domain \( \Omega = (1, \omega] \).

As the parameter of \( x^* \) corresponding to the interior edge is 1, \( \varphi_T(x^*) \) belongs to the intersection of the tree phylogenetic varieties \( V_{1234} \cap V_{1324} \cap V_{1423} \) (see also Lemma 4.1), for that reason it is natural to ask whether if \( x^* = (k(k, m), 1, k(k, m), 1, 1) \) is also a local minimum of the optimization problem 6.1 for \( T = 12 \cap V_T \).

The following proposition (proved in Appendix A Proposition A.1) claims that \( \hat{x}(k, m) \) is indeed a real number. The computations in this section and in the Appendix have been done with SageMath version 8.6.

Proposition 6.2. \( \hat{x}(k, m) \) is a well-defined real number for all \( k \in [-1/3, 1) \) and \( m \in \Omega := (1, \omega] \), where \( \omega = \frac{4}{9} + \frac{11}{27} \sqrt{69 + 16\sqrt{3}} + \sqrt{\frac{69 + 16\sqrt{3}}{243}} \approx 1.734 \).

Moreover, \( \nabla g_T(x) = (0, \ldots, \hat{1}, \ldots, 0)^t \) for all \( i \) and for every \( x \). Therefore condition (i),

\[-\nabla f_{1234}(x^*) = \mu_{1,2} \nabla g_{12}(x^*) + \mu_{1,4} \nabla g_{14}(x^*) + \mu_{1,5} \nabla g_{15}(x^*),\]

is equivalent to

\[ \left( 0, \frac{\partial f_{1234}}{\partial x_2} \bigg|_{x^*}, 0, \frac{\partial f_{1234}}{\partial x_4} \bigg|_{x^*}, \frac{\partial f_{1234}}{\partial x_5} \bigg|_{x^*} \right)^t = -(0, \mu_{1,2}, 0, \mu_{1,4}, \mu_{1,5})^t, \]
which implies that necessarily

\[
\begin{align*}
\mu_{1,2} &= -\left. \frac{\partial f_{12|34}}{\partial x_2} \right|_{x^*}, \\
\mu_{1,4} &= -\left. \frac{\partial f_{12|34}}{\partial x_4} \right|_{x^*}, \\
\mu_{1,5} &= -\left. \frac{\partial f_{12|34}}{\partial x_5} \right|_{x^*}.
\end{align*}
\]

Because of condition \((iii)\), to conclude it is enough to show that these partial derivatives are negative. This is proven in part \(a)\) of Lemma \(A.5\), Lemma \(A.6\) and Lemma \(A.7\) of the Appendix. Moreover, \(x^*\) is a minimum because according to Lemma \(A.9\ a)\) (see Appendix), \(x^*\) is a minimum of the function \(f_{12|34}\) restricted to the boundary \(x_2 = x_4 = x_5 = 1\).

If \(\hat{x}(k,m)\) is greater than 1, by the KKT conditions and the same reasoning as before we need to prove that \(\left. \frac{\partial f_{12|34}}{\partial x_i} \right|_{x^*}\) is negative for every \(i\), since any partial derivative of \(f_{12|34}\) vanishes on \(x^*\). This is proven in part \(b)\) of Lemma \(A.5\), Lemma \(A.6\), Lemma \(A.7\) and Lemma \(A.9\) of the Appendix. Therefore \(x^*\) is a local optimum.

The proof for the topology \(13|24\) follows directly from the previous results since the function \(f_{13|24}\) satisfies \(\left. \frac{\partial f_{13|24}}{\partial x_i} \right|_{x^*} = \left. \frac{\partial f_{12|34}}{\partial x_i} \right|_{x^*}\) for \(i = 2, 4\) and \(\left. \frac{\partial f_{13|24}}{\partial x_5} \right|_{x^*}\) is also negative by Lemma \(A.8\).

\[
6.2. \text{Global minimum.}
\]

\textbf{Conjecture 6.5.} Let \(P_0 := \varphi_T(k_0, 1, k_0, 1, m_0)\). If \(k_0 \in [-1/3, 1]\) and \(m_0 \in \Omega\), then

\[
d(P_0, \mathcal{V}_T^+ = \min d(P_0, \varphi_T(\tilde{x}(k_0, m_0), 1, \tilde{x}(k_0, m_0), 1, 1))\).
\]

\textbf{Remark 6.6.} We have tested the conjecture for 1000 pairs of parameters \((k, m)\) randomly chosen on the region \((0,1/4) \times (1,3/2)\) in order to simulate points close to the LBA phenomenon. Every experiment has verified that the global minimum of the problem is the point \(x^* = (\kappa(k,m), 1, \kappa(k,m), 1, 1)\), where \(\kappa(k)\) is defined as in \([4]\) and which was proved to be a local minimum. A list of the tested parameters \(k\) and \(m\) can be found in \([3]\).

In the cases where the conjecture is satisfied, we have:

\textbf{Theorem 6.7.} Let \(k_0 \in [-1/3, 1]\), \(m_0 \in \Omega\) and assume that \(P_0 := \varphi_T(k_0, 1, k_0, 1, m_0) \in \mathcal{V}_T\), satisfies \(d(P_0, \mathcal{V}_T^+) = d(P_0, \varphi_T(\tilde{x}(k_0, m_0), 1, \tilde{x}(k_0, m_0), 1, 1))\) with \(\tilde{x}(k_0, m_0) \neq 1\). Then, if \(P\) is close enough to \(P_0\) and \(T' \neq T\) is another tree in \(T\), its closest point in \(\mathcal{V}_T^+\) belongs also to \(\mathcal{V}_T^+\). In particular,

\[
d(P, \mathcal{V}_T^+) \geq d(P, \mathcal{V}_T^+).
\]

\textbf{Proof.} Let \(W_{P_0} := \left\{ \varphi_T(x) \mid x \in \mathcal{D} \text{ and } \left. \frac{\partial f_T}{\partial x_i} \right|_{x} = 0 \forall i \in [1, \ldots, 5] \right\}\) be the image of the set of critical points of \(f_T\) that satisfies the problem constrains. Write \(\mathcal{B}_{x=1}\mathcal{V}_T\) for the set of border points \(\varphi_T(x) \in \mathcal{V}_T^+\) with \(x = (x_1, \ldots, x_4, 1)\). If \(P_0^+\) is the closest point in \(\mathcal{V}_T^+\) to \(P_0\), then \(P_0^+ \in \mathcal{B}_{x=1}\mathcal{V}_T\ \backslash W_{P_0}\) because the hypothesis \(P_0^+ = \varphi_T(\tilde{x}(k_0, m_0), 1, \tilde{x}(k_0, m_0), 1, 1)\) implies that the partial derivatives are non-zero (see Lemmas \(A.5\), \(A.6\) and \(A.7\)). Define
\[ g(P) := d(P, W_P) - d(P, B_{x_5=1}V_T) \]. Therefore \( g(P_0) > 0 \) and \( g(P) \) is also positive if \( P \) is close enough to \( P_0 \). It follows that \( d(P, W_P) > d(P, B_{x_5=1}V_T) \) and therefore

\[
\min_{Q \in V_T} d(P, Q) = \min_{Q \in B_{x_5=1}V_T} d(P, Q).
\]

Finally, \( d(P, V_T^+) \leq \min_{Q \in B_{x_5=1}V_T} d(P, Q) = \min_{Q \in B_{x_5=1}V_T} d(P, Q) = d(P, V_T^+) \) since \( B_{x_5=1}V_T = B_{x_5=1}V_T \subset V_T^+ \cap V_T^+ \).

7. Study on simulated data

In this section we simulate points close to a given phylogenetic variety and we compute its distance to the stochastic part of this variety as well as to the other phylogenetic varieties (distinguishing also the stochastic part of the varieties). We do this in the setting of long branch attraction of the previous section and for balanced trees. We cannot do this theoretically because, even if we have found a local minimum for the long branch attraction setting (Theorem 6.4), we cannot warranty that it is global and also because we do not know exactly the distance when the input does not lie on the variety. To do the computations of this section we use Algorithm 1.

We consider a 4-leaf tree 12|34 with JC69 matrices. Suppose \( k_a \) and \( k_b \) are the eigenvalues of matrices at the exterior edges and \( M \) is a JC69 matrix at the interior edge, with eigenvalue \( m \) that takes values in the interval \([0.94, 1.06]\) (see Figure 4). These trees represent points in \( V_{12|34} \) that range from the stochastic part of the variety \( V_{12|34}^+ \) (that is \( m \leq 1 \)) to the non-stochastic part \((m > 1)\). For each set of parameters we considered 100 data points, each corresponding to the observation of 10000 independent samples from the corresponding multinomial distribution \( \varphi_T(k_a, k_b, k_a, k_b, m) \).

\[
\text{Figure 4. Tree } 12|34 \text{ with distribution } P = \varphi(k_a, k_b, k_a, k_b, m)
\]

For each data point \( P \) generated as above and for each tree \( T \in \mathcal{T} \), we have computed the distance of \( P \) to the stochastic part of the variety \( V_T^+ \), \( d(P, V_T^+) \) using Algorithm 1 and we have also computed the the distance to the complete variety, \( d(P, V_T) \). These computations have been performed for the three tree topologies 12|34, 13|24 and 14|23.

For each set of parameters \( k_a, k_b \) and \( m \) we have plotted, the average of each of these distances computed from the 100 data points. In each graphic we have fixed \( k_a \) and \( k_b \) and let \( m \) vary in the \( x \)-axis from 0.94 to 1.06; the \( y \)-axis represents the distance. The grey background part of the plots represent the region of data points sampled from non the stochastic part of the variety, whereas the white part represents the stochastic part.
Figure 5. Eigenvalues $k_a = 0.37$ and $k_b = 0.87$. On the left: distance to the phylogenetic varieties $\mathcal{V}_T$. On the right: distance to the stochastic part of the varieties $\mathcal{V}_T^+$.

Figure 6. Eigenvalues $k_a = k_b = 0.51$. On the left: distance to the phylogenetic varieties $\mathcal{V}_T$. On the right: distance to the stochastic part of the varieties $\mathcal{V}_T^+$.

The first plot (Figure 5) represents trees on the long branch attraction phenomena and the second one (Figure 6) represent balanced trees. In both cases we observe a similar behaviour. The distance to the variety $\mathcal{V}_{12|34}$ is in general smaller for all values of $m$ (except when we are really close to the intersection). But if we observe the distance to the stochastic variety we see that when $m > 1$ the distance to $\mathcal{V}_T^*_{12|34}$ becomes grater than the distance to the other stochastic varieties and this confirm the inequality of Theorem 6.7. However, for $m < 1$ the distance to $\mathcal{V}_T^*_{12|34}$ is always the smallest.
The different performance on the two plots of the distances to $V_{13|24}^+$ and $V_{14|23}^+$ are due to the shapes of the trees that we are considering. On the case of balance trees we see that the distances to $V_{13|24}^+$ and $V_{14|23}^+$ are almost equal.

Every simulation performed has showed us that, when $m > 1$, the closest point to $P$ in $V_{12|34}^+ \cap V_{13|24}^+ \cap V_{14|23}^+$ belongs to the varieties intersection, i.e. $P_{12|34}^+ \in V_{12|34}^+ \cap V_{13|24}^+ \cap V_{14|23}^+$. However, this is not true when we compute the closest point to $T$ for $T \neq 12|34$. In the case of long branch attraction (see Figure 5) the closest point $P_{14|23}^+ \in V_{14|23}^+$ to $P$ is always at the interior of the stochastic variety $V_{14|23}^+$ whether for $T = 13|24$, the closest point to $P$ is in the interior of $V_{13|24}$ approximately half the time.

These simulations verify that if $P \in \mathbb{R}^{44}$ is a distribution satisfying $d(P, V_{12|34}) < \min\{d(P, V_{13|24}), d(P, V_{14|23})\}$ it is possible that $d(P, V_{12|34}^+) > \min\{d(P, V_{13|24}^+), d(P, V_{14|23}^+)\}$. This provides an affirmative answer to the Question 1 posed at the beginning of the paper. This suggests that considering the stochastic part of phylogenetic varieties and the resulting semi-algebraic constraints needed to describe them may be an interesting strategy for phylogenetic reconstruction in the long branch attraction setting, and also for balanced trees. However, as it has become evident throughout this paper, to deal with both algebraic and semi-algebraic conditions is not an easy task, and more work is needed in order to design practical methods for phylogenetic inference under more general evolutionary models than the models used here.

7.1. Computations. The computations were performed on a machine with 10 Dual Core Intel(R) Xeon(R) Silver 64 Processor 4114 (2.20 GHz, 13.75M Cache) equipped with 256 GB RAM running Ubuntu 18.04.2. We have used Macaulay2 version 1.3 and SageMath version 8.6.

REFERENCES

[1] Allman, E. S., Degnan, J. H., and Rhodes, J. A. Species tree inference by the star method and its generalizations. *Journal of Computational Biology* 20, 1 (2013), 50–61.

[2] Allman, E. S., Kubaš, L. S., and Rhodes, J. A. Split Scores: A Tool to Quantify Phylogenetic Signal in Genome-Scale Data. *Systematic Biology* 66, 4 (2017), 620–636.

[3] Allman, E. S., and Rhodes, J. A. Phylogenetic invariants of the general Markov model of sequence mutation. *Math. Biosci.* 186 (2003), 113–144.

[4] Allman, E. S., and Rhodes, J. A. Mathematical models in biology, an introduction. Cambridge University Press, January 2004. ISBN 0-521-52586-1.

[5] Allman, E. S., and Rhodes, J. A. Quartets and parameter recovery for the general Markov model of sequence mutation. *Applied Mathematics Research Express* 2004 (2004), 107–132.

[6] Allman, E. S., and Rhodes, J. A. Phylogenetic invariants. In *Reconstructing Evolution*, O. Gascoigne and M. A. Steel, Eds. Oxford University Press, 2007.

[7] Allman, E. S., and Rhodes, J. A. The identifiability of covarion models in phylogenetics. *IEEE ACM Trans. Comput. Biol. Bioinformatics* 6 (2009), 76–88.

[8] Allman, E. S., Rhodes, J. A., and Taylor, A. A semialgebraic description of the general markov model on phylogenetic trees. *SIAM Journal on Discrete Mathematics* 28 (12 2012).

[9] Bosma, W., Cannon, J., and Playoust, C. The Magma algebra system. I. The user language. *J. Symbolic Comput.* 24, 3–4 (1997), 235–265. Computational algebra and number theory (London, 1993).

[10] Casanellas, M., and Fernández-Sánchez, J. Performance of a new invariants method on homogeneous and nonhomogeneous quartet trees. *Mol. Biol. Evol.* 24 (2007), 288–293.

[11] Casanellas, M., and Fernández-Sánchez, J. Geometry of the Kimura 3-parameter model. *Advances in Applied Mathematics* 41, 3 (2008), 265–292.

[12] Casanellas, M., Fernández-Sánchez, J., and Michalek, M. Low degree equations for phylogenetic group-based models. *Collectanea Mathematica* 66, 2 (2015), 203–225.
[13] Chifman, J., and Kubatko, L. Quartet Inference from SNP Data Under the Coalescent Model. *Bioinformatics* 30, 23 (2014), 3317–3324.

[14] Chifman, J., and Kubatko, L. Identifiability of the unrooted species tree topology under the coalescent model with time-reversible substitution processes, site-specific rate variation, and invariable sites. *Journal of Theoretical Biology* 374 (2015), 35–47.

[15] Cox, D. A., Little, J., and O’Shea, D. *Ideals, Varieties, and Algorithms: An Introduction to Computational Algebraic Geometry and Commutative Algebra, (Undergraduate Texts in Mathematics).* Springer-Verlag, Berlin, Heidelberg, 2007.

[16] Draisma, J., Horobet, E., Ottaviani, G., Sturmfels, B., and Thomas, R. The euclidean distance degree of an algebraic variety. *Foundations of Computational Mathematics* (2015), 1–51.

[17] Draisma, J., and Kuttler, J. On the ideals of equivariants tree models. *Mathematische Annalen* 344 (2009), 619–644.

[18] Evans, S. N., and Speed, T. P. Invariants of some probability models used in phylogenetic inference. *Ann. Stat.* 21(1) (1993), 355–377.

[19] Fernández-Sánchez, J., and Casanellas, M. Invariant versus classical quartet inference when evolution is heterogeneous across sites and lineages. *Systematic Biology* 65, 2 (2016), 280–291.

[20] Grayson, D. R., and Stillman, M. E. *Macaulay2, a software system for research in algebraic geometry.* Available at [http://www.math.uiuc.edu/Macaulay2/](http://www.math.uiuc.edu/Macaulay2/).

[21] Gross, E., Davis, B., L. Ho, K., J. Bates, D., and A. Harrington, H. Numerical algebraic geometry for model selection and its application to the life sciences. *Journal of the Royal Society Interface* 13 (10 2016).

[22] Gross, E., Petrovic, S., and Verschelde, J. Interfacing with phcpack. *Journal of Software for Algebra and Geometry* 5 (01 2013), 20–25.

[23] Jukes, T., and Cantor, C. Evolution of protein molecules. *In Mammalian Protein Metabolism* (1969), 21–132.

[24] Kimura, M. Estimation of evolutionary distances between homologous nucleotide sequences. *Proc. Natl. Acad. Sci.* 78 (1981), 1454–1458.

[25] Klaere, S., and Liesbcher, V. An algebraic analysis of the two state markov model on tripod trees. *Mathematical Biosciences* 237, 1 (2012), 38 – 48.

[26] Kosta, D., and Kujbas, K. Maximum likelihood estimation of symmetric group-based models via numerical algebraic geometry. *Bulletin of Mathematical Biology* 81, 2 (2019), 337–360.

[27] Kreinin, A., and Sidelnikova, M. Regularization algorithms for transition matrices. *Algo Research Quarterly* 4 (2001), 2340.

[28] Lake, J. A. A rate-independent technique for analysis of nucleic acid sequences: evolutionary parsimony. *Mol. Biol. Evol.* 4 (1987), 167–191.

[29] Matsen, F. A. Fourier transform inequalities for phylogenetic trees. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 6, 1 (2009), 89–95.

[30] Michelot, C. A finite algorithm for finding the projection of a point onto the canonical simplex of rn. *J. Optim. Theory Appl.* 50, 1 (July 1986), 195–200.

[31] The SAGE Developers. *SageMath, the Sage Mathematics Software System (Version 8.6)*, 2019. [https://www.sagemath.org](https://www.sagemath.org).

[32] Verschelde, J. Phcpack: a general-purpose solver for polynomial systems by homotopy continuation. *ACM Trans. Math. Softw.* 25, 2 (1999), 251–276.

[33] Zwierink, P., and Smith, J. Q. Implicit inequality constraints in a binary tree model. *Electronic Journal of Statistics* 5 (2011), 1276–1312.
A.1. Proof of Proposition 6.2

Proposition A.1. $\tilde{x}(k, m)$ is a real number for all $k \in I := [-1/3, 1]$ and $m \in \Omega := (1, \omega]$, where $\omega = \frac{4}{9} + \frac{11}{27 \sqrt[3]{69 + 16\sqrt{3}}} + \sqrt[3]{\frac{69 + 16\sqrt{3}}{243}} \approx 1.734$. 

Proof. To prove this result we need to verify that $\gamma(k, m) \neq 0$ and $\alpha(k, m) \geq 0$, for $k \in I$, $m \in \Omega$. Unless noted otherwise we will assume $m > 1$ during all this reasoning.

We first study when the denominator of $\kappa$ vanishes. $\gamma(k, m) = 0$ if and only if $\gamma(k, m)^3 = 9k(3m + 1) + \sqrt[3]{\alpha(k, m)} = 0$. It is equivalent to 

\begin{equation}
9k(3m + 1) = -\sqrt[3]{\alpha(k, m)}
\end{equation}

Then $\alpha(k, m) - (9k(3m + 1))^2 = - (9k^2m + 3k^2 - 4)^3 = 0$ if and only if $k = \pm \frac{2}{\sqrt{9m + 3}}$. Only the negative solution of $k$ satisfies equation (7). Note that $k = -\frac{2}{\sqrt{9m + 3}}$ is always negative and it will be greater than $-1/3$ if and only if $m < \frac{11}{3}$. Therefore, for all $k \in [-1/3, 1]$ and $m < \frac{11}{3}$, $\kappa(k, m)$ is a real number since $\gamma(k, m)$ is never zero. \hfill \Box

The following lemma finishes the proof.

Lemma A.2. $\alpha(k, m) \geq 0 \ \forall k \in I, \ m \in \Omega$

Proof. Consider $\alpha_m(k) := \alpha(k, m)$ as a function of $k$:

$$
\alpha_m(k) = \frac{(-729m^3 - 729m^2 - 243m - 27)k^6 + (972m^2 + 648m + 108)k^4}{a(m)} + \frac{(729m^2 + 54m - 63)k^2 + 64}{c(m)}
$$

It is an even function in $k$ ($\alpha_m(k) = \alpha_m(-k)$) and it goes to minus infinity when $k$ goes to $\pm \infty$. Moreover it is a polynomial of degree 6 in $k$ with polynomials in $m$ as coefficients.

This function has a local minimum at $k = 0$ since

$$
\begin{align*}
\alpha_m(k) &= a(m)k^6 + b(m)k^4 + c(m)k^2 + d \quad \text{and} \quad \alpha_m(0) = d = 64 > 0, \\
\alpha_m'(k) &= 6a(m)k^5 + 5b(m)k^3 + 2c(m)k \quad \text{and} \quad \alpha_m'(0) = 0, \\
\alpha_m''(k) &= 30a(m)k^4 + 10b(m)k + 2c(m) \quad \text{and} \quad \alpha_m''(0) = 2(729m^2 + 54m - 63) > 0 \quad \text{for} \ m > 1.
\end{align*}
$$

Since $\alpha_m(k)$ is an even polynomial in $k$ with one positive minimum at $k = 0$ and limit to $-\infty$ when $k$ goes to $\pm \infty$, its number of real roots will be even and at least two. Suppose $\alpha_m(k)$ has 4 or 6 real roots, then the number of local extremes of $\alpha_m(k)$ should be at least 7, but $\alpha_m'(k)$ has degree 5, and therefore it has at most 5 roots. Therefore $\alpha_m(k)$ will only have 2 real roots (one positive and one negative) and a minimum at $k = 0$.

By Descartes rule we can count the number of positive (and negative) roots of $\alpha_m(k)$: Let $p(x)$ be a polynomial of one variable in descending power order. Then the number
of positive roots (counted with multiplicity) of \( p(x) \) is either the number of sign changes between consecutive nonzero coefficients or is less than it by an even number.

Trivially we see that for any \( m > 1 \), \( a(m) = -729m^3 - 729m^2 - 243m - 27 < 0 \), \( b(m) = 972m^2 + 648m + 108 > 0 \), \( c(m) = 729m^2 + 54m - 63 > 0 \) and \( d > 0 \), therefore \( \alpha_m(k) \) has exactly one positive (and by symmetry one negative) root.

We want to see now that the root of \( \alpha_m(k) \) does not belong to \( I \) if \( m \in \Omega \). Define \( m_1 := 1 \) and \( m_2 := \omega \approx 1.734 \). Then, \( \alpha_{m_1}(k) = -1728k^6 + 1728k^4 + 720k^2 + 64 \) is zero if and only if \( k = \pm k_1 := \pm \frac{2\sqrt{3}}{3} \approx \pm 1.154 \not\in I \).

Moreover the roots of \( \alpha_{m_2}(k) = 0 \) are \( \pm k_2 := \pm 1 \).

![Figure 7](image)

It remains to see that for any \( \hat{m} \in \Omega \), the positive root of \( \alpha_{\hat{m}}(k) = 0 \) belongs to \( [k_2, k_1] \). To do it, first consider \( \alpha(k,m) \) as a function of \( m \),

\[
\alpha_k(m) = \left( -729k^6 \right) m^3 + 243 \left( -3k^6 + 4k^4 + 3k^2 \right) m^2 + 27 \left( -9k^6 - 24k^4 - 2k^2 \right) m \\
-27k^6 + 108k^4 - 63k^2 + 64.
\]

This exhibits \( \alpha_k(m) \) as a degree 3 polynomial in \( m \) and it has a unique real root since it has negative discriminant

\[
D_{\alpha_k(m)} = 18a(k)b(k)c(k)d(k) - 4b(k)^3d(k) + b(k)^2c(k)^2 - 4a(k)c(k)^3 - 27a(k)^2d(k)^2
\]

\[
= -99179645184(k^6 + 3k^8)
\]

for all \( k \) different from zero. The region where this real root is positive can be determined by using the Descartes rule. Let us study the sign of the coefficients:

- \( a(k) = -729k^6 < 0 \) \( \forall k \neq 0 \).
- \( b(k) = 243(-3k^6 + 4k^4 + 3k^2) = 0 \) if and only if \( k^2(-3k^4 + 4k^2 + 3) = 0 \). The real solutions of this polynomial are \( k = 0 \), \( k = r_b := \sqrt{\frac{2 + \sqrt{13}}{3}} \) and \( k = -r_b \).

Evaluating at \( b(k) \) we have \( b(k) < 0 \) for \( |k| > r_b \) and \( b(k) > 0 \) for \( -r_b < k < r_b \) and \( k \neq 0 \).
Lemma A.3. Let \( f(x) = 27(-9k^6 - 24k^4 - 2k^2) \) if and only if \( k^2(-9k^4 + 24k^2 + 2) = 0 \). The real solutions of \( f(k) \) are \( k = 0, k = r_c := +\sqrt{\frac{4}{3} + 2} \) and \( k = -r_c \). Again, evaluating the polynomial we have \( f(k) < 0 \) for \( |k| > r_c \) and \( f(k) > 0 \) for \( -r_c < k < r_c \) and \( k \neq 0 \).

Lemma A.4. Let \( d(k) = -27k^6 + 108k^4 - 63k^2 + 64 \). The roots of \( d(k) = 0 \) are \( k = r_d := \sqrt{\frac{4}{3} + \sqrt{2 - \sqrt{3 + \sqrt{2 + \sqrt{3}}}}} \) and \( k = -r_d \). Thus, \( d(k) > 0 \) when \( -r_d < k < r_d \) and \( d(k) < 0 \) if \( |k| > r_d \).

For any \( k \in [-r_d, r_d] \) there is only one sign difference between consecutive coefficients, since \( r_b < r_c < r_d \). Therefore the real root of \( \alpha_k(k) \) will be positive for any \(-r_d < k < r_d \) different from zero, and negative if \( |k| > r_d \). Since \( r_d \approx 1.8786 \) and \( k_2 = 1 \), \( \alpha_k(k) \) always has one positive root for any \( k \in [k_1, k_2] \).

As a consequence of the following lemma the positive root of \( \alpha_{\hat{m}}(k) \) is in \([k_2, k_1]\) for any \( \hat{m} \in [m_1, m_2] \). Therefore \( \alpha(k, m) \) is never zero for any \( k \in I \) or \( m \in \Omega \) and, since it is a continuous function, its sign is constant on this domain. Evaluating the function we check that \( \alpha(k, m) \) is positive on the defined region.

**Lemma A.3.** Let \( k : [m_1, m_2] \to [k_2, k_1] \) be the positive solution of \( \alpha_{\hat{m}}(k) = 0 \) (so that \( \alpha(k, m) = 0 \) \( \forall m \in [m_1, m_2] \)). Then \( \alpha(k, m) \) is continuous and injective.

**Proof** Ass observed in the proof of Lemma A.2, \( \alpha_k(k) \) has one and only one real and positive root for any \( m > 1 \). Therefore \( \alpha(k, m) \) is well defined and continuous by the implicit function Theorem.

Recall that \( k(+m_1) > k(+m_2) \) but \( m_1 < m_2 \). Then consider the following two cases:

(i) \( k(m) \) is strictly increasing, therefore it is injective.

(ii) \( k(m) \) is not strictly decreasing. Since it is continuous and \( k(m_1) > k(m_2) \) there exist some \( m', m'' \in [m_1, m_2] \) such that \( k(m') = k(m'') = k \). Therefore \( \alpha(k(m'), m') = \alpha(k(m''), m'') = 0 \) and \( \alpha(k, m') = \alpha(k, m'') = 0 \). Moreover \( \alpha_k(m') = \alpha_k(m'') = 0 \). This is not possible since, as noted in the proof of Lemma A.2, \( \alpha_k \) has a unique real and positive root for any \( k \).

**A.2. Proof of Theorem 6.4.** The proofs of the following Lemmas will be all divided into two parts. On the first one we assume \( \hat{x}(k, m) < 1 \) and on the other one \( \hat{x}(k, m) \) is assumed to be greater or equal than 1. For that reason, we start studying for which parameters \( k \) and \( m \), \( \hat{x}(k, m) \) equals 1.

**Lemma A.4.** \( \hat{x}(k, m) \) equals 1 if and only if \( m = m^* := \frac{-3k^2 - k + 16}{3k(3k + 1)} \). Moreover, \( \hat{x}(k, m) > 1 \) if and only if \( m > m^* \).
Lemma A.5. $\partial f_{m}$ only if (9)

\begin{align*}
\text{(9)}
\begin{cases}
p(x) := x - 1 = 0 \\
p(z(x, g, k, m)) := 36xg - 36g^2 - 9k^2m + 3k^2 + 4 = 0 \\
p_\gamma(g, a, k, m) := 216g^3 - 9k(3m + 1) - a = 0 \\
p_\alpha(a, k, m) := a^2 - \alpha(k, m) = 0
\end{cases}
\end{align*}

Proof. Consider the new variables $x$, $g$ and $a$ that will allow us to make explicit the relations of $\hat{x}(k, m)$, $\gamma(k, m)$ and $\alpha(k, m)$. Then $\hat{x}(k, m) - 1$ is zero if and only if $(k, m)$ is a solution of the system of equations:

\begin{align*}
\begin{cases}
p(x) := x - 1 = 0 \\
p(z(x, g, k, m)) := 36xg - 36g^2 - 9k^2m + 3k^2 + 4 = 0 \\
p_\gamma(g, a, k, m) := 216g^3 - 9k(3m + 1) - a = 0 \\
p_\alpha(a, k, m) := a^2 - \alpha(k, m) = 0
\end{cases}
\end{align*}

Polynomials $p_\hat{x}$, $p_\gamma$ and $p_\alpha$ stand for the relations introduced in (4), (5) and (6) respectively. Define the ideal $I := (p(x), p_\hat{x}(x, g, k, m), p_\gamma(x, g, a, k, m), p_\alpha(a, k, m))$ and compute the elimination ideal $I \cap \mathbb{C}[k, m]$. According to Lemma 1 and Theorem 3 in section 3.2 of [15], the variety $V(I \cap \mathbb{C}[k, m])$ is the smallest algebraic variety containing the points $(k, m)$ that correspond to points in $V(I)$. However this inclusion is strict and there are points $(k, m) \in V(I \cap \mathbb{C}[k, m])$ that do not expand to solutions of (9).

In this case, the ideal $I \cap \mathbb{C}[k, m]$ is generated by the polynomial:

\[ j(k, m) = (9k^2m + 3k^2 - 4)^3\left(9k^2m + 3k^2 + 3km + k - 16\right). \]

Studying the solutions of $j(k, m) = 0$ one can see that polynomials on (9) vanish if and only if $m = m^*$. Moreover by checking at any point such that $m > m^*$ we prove that $\hat{x}(k, m) > 1$ if and only if $m > m^*$.

Lemma A.5. \left. \frac{\partial f_{1234}}{\partial x_2} \right|_{x^*} \text{ is negative for all } (k, m) \in I \times \Omega.

Proof. The proof falls naturally into two cases.

a) Suppose $\hat{x} < 1$:

By definition, $\kappa(k, m) = \hat{x}(k, m)$ in this case. Therefore,

\[ \left. \frac{\partial f_{1234}}{\partial x_2} \right|_{x^*} = 54\hat{x}^4 + (-36k^2m - 18k^2 + 36)\hat{x}^2 - (30km + 6k)\hat{x} - 6m + 6 \]

To prove that this function is negative we prove that it never vanishes on $I \times \Omega$ and is negative for a particular value in that region. \left. \frac{\partial f_{1234}}{\partial x_2} \right|_{x^*} \text{ is zero if and only if the following polynomials vanish:}

\begin{align*}
\text{(10)}
\begin{cases}
p(x, k, m) = 54x^4 + (-36k^2m - 18k^2 + 36) x^2 - (30km + 6k) x - 6m + 6, \\
p(z(x, g, k, m)), \\
p_\gamma(g, a, k, m), \\
p_\alpha(a, k, m)
\end{cases}
\end{align*}

where $p_\hat{x}(x, g, k, m)$, $p_\gamma(g, a, k, m)$ and $p_\alpha(a, k, m)$ are defined as in (9).

We consider the ideal $I = (p(k, m, x), p_\hat{x}(k, m, x, g), p_\gamma(k, m, x, g, a), p_\alpha(k, m, a))$ and we compute the elimination ideal $I \cap \mathbb{C}[k, m]$ which turns out to be generated by exactly

The idea and arguments presented in the following proof will be also used in the remaining proofs of this section. They are based on basic concepts and results on Elimination Theory, good general reference here is the Chapter 3 of [15].
one polynomial,  
\[ j(k,m) = (m-1)(3k^2+1)(9k^2m+3k^2-4)^3(81k^6m^3-27k^6m^2-45k^6m-9k^6+39k^4m^3 \\
+547k^4m^2+469k^4m+97k^4-1312k^2m^2-1120k^2m-256k^2-768m^2) \]

The polynomial \( j(k,m) \) is zero if and only if at least one of these polynomial vanishes:

\[ j_1(k,m) = m - 1 \]
\[ j_2(k,m) = 3k^2 + 1 \]
\[ j_3(k,m) = 9k^2m + 3k^2 - 4 \]
\[ j_4(k,m) = 81k^6m^3 - 27k^6m^2 - 45k^6m - 9k^6 + 39k^4m^3 + 547k^4m^2 \\
+ 469k^4m + 97k^4 - 1312k^2m^2 - 1120k^2m - 256k^2 - 768m^2 \]

The first polynomial is zero when \( m = 1 \), but \( 1 \not\in \Omega \). The second one has no real solutions in \( k \). Note that \( j_3(k,m) \) is zero when \( k^\pm(m) = \pm 2 \sqrt{9m+3} \). However \( k^- \not\in I \) if \( m \in \Omega \) (see part (i) of the proof of Lemma 6.2) and \( k^+(m) \) does not generate a solution of \([10] \). The case of \( j_4 \) is not that simple. Consider it as a function of \( m \):

\[ j_{4,k}(m) = \frac{\left(81k^6 + 39k^4\right)m^3 + \left(-27k^6 + 547k^4 - 1312k^2 - 768\right)m^2 + \\
\left(-45k^6 + 469k^4 - 1120k^2\right)m + \left(-9k^6 + 97k^4 - 256k^2\right)}{d(k)} \]

The discriminant (see [5]) of \( j_{4,k}(m) \) is

\[ D_{j_{4,k}}(k) = 49152k^2(64 + 115k^2 - 38k^4 + 3k^6)(-2304 + 1020k^2 - 340k^4 + 39k^6) \]
\[ = -49152k^2(\sqrt{6} - k)(\sqrt{6} + k)(384 - 106k^2 + 39k^4)(64 + 115k^2 - 38k^4 + 3k^6)^2 \]

The polynomial \( D_{j_{4,k}}(k) \) has three real roots at \( k = 0 \) and \( k = \pm \sqrt{6} \sim 2.449 \). Since \( D_{j_{4,k}}(-1) = D_{j_{4,k}}(1) = -1615457157120 < 0 \) we conclude \( D_{j_{4,k}}(k) \leq 0 \forall k \in I \) and hence \( j_{4,k}(m) \) only has one real root in this interval. Evaluating at \( m = 1 \) and \( m = 2 \) we get,

- \( j_{4,k}(1) = 384(3k^4 - 7k^2 - 2) = 0 \) if and only if \( k = \pm \sqrt{\frac{7 + \sqrt{13}}{6}} = \pm 1.609 \). Moreover \( j_{4,k}(1) < 0 \forall k \in I \) since \( j_{4,k}(0,1) = -768 < 0 \).
- \( j_{4,k}(2) = 441k^6 + 3535k^4 - 7744k^2 - 3072 \) is zero for \( k \sim \pm 1.4399 \). At \( k = 0 \) we have \( j_{4,k}(0,2) = -3072 < 0 \), then \( j_{4,k}(2) \) is also negative \( \forall k \in I \).

This clearly forces the root of \( j_{4,k}(m) \) to not be in \( \Omega \) and consequently \( V(I \cap \mathbb{C}[k,m]) \cap I \times \Omega = \emptyset \). Since \( f_{1234} \) is continuous and well defined in \( I \times \Omega \) it may be concluded that \( f_{1234} \) has the same sign in all the domain. Evaluating at any point \((k,m) \in I \times \Omega\) we conclude that \( \frac{\partial f}{\partial x_2}(x^*(k,m)) \) is negative on this region.

b) Suppose that \( \tilde{x} \geq 1 \), then we prove that \( \frac{\partial f}{\partial x_2} \mid_{x=(1,1,1,1,1)} < 0 \):
The function \( \frac{\partial f_{1234}}{\partial x_2} \bigg|_1 = -18k^2 - 6(6k^2 + 5k + 1)m - 6k + 96 \) is negative if and only if \( m > \frac{-3k^2 - k + 16}{6k^2 + 5k + 1} \). Moreover, \( \frac{-3k^2 - k + 16}{6k^2 + 5k + 1} < m^* \) for all \( k < 5/3 \) and therefore \( \frac{\partial f_{1234}}{\partial x_2} \bigg|_1 \) is negative for all \( m > m^* \).

Lemma A.6. \( \frac{\partial f_{1234}}{\partial x_4} \bigg|_{x^*} \) is negative for all \( (k, m) \in I \times \Omega \).

Proof. Computing the partial derivative and substituting we get \( \frac{\partial f_{1234}}{\partial x_4} \bigg|_{x^*} = \frac{\partial f_{1234}}{\partial x_2} \bigg|_{x^*} \). This follows from the symmetry on \( f_{1234} \) and on \( x^* \). Therefore, Lemma A.6 is a consequence of Lemma A.5.

Lemma A.7. \( \frac{\partial f_{1234}}{\partial x_5} \bigg|_{x^*} \) is negative for all \( (k, m) \in I \times \Omega \).

Proof. a) Suppose \( \hat{x} < 1 \):

\[
\frac{\partial f_{1234}}{\partial x_5} \bigg|_{x^*} = -54\hat{x}^4 + (-54k^2m + 36)\hat{x}^2 - 36km\hat{x} - 6m + 6.
\]

In this case consider the ideal \( I = (p(x, k, m), p_2(x, g, k, m), p_3(x, g, a, k, m), p_4(a, k, m)) \) where \( p(x, k, m) = -54x^4 + (-54k^2m + 36)x^2 - 36kmx - 6m + 6 \). The ideal \( I \cap \mathbb{C}[k, m] \) is generated by the polynomial,

\[
j'(k, m) = j_1(k, m) \cdot j_2(k, m) \cdot j_3(k, m) \cdot j_4(k, m),
\]

where \( j_1(k, m) = 81k^4m^3 + (-27k^4 - 288k^2 - 256)m^2 + (-45k^4 - 96k^2)m - 9k^4 \) and \( j_1, j_2 \) and \( j_3 \) are defined as in (11), (12) and (13). We only need to study the intersection of \( j_4' \) with \( I \times \Omega \). Taking \( j_4' \) as a function of \( m \) we compute its discriminant,

\[
D_{j_4,k}(k) = -442368k^6(2 + 3k^2)(128 + 18k^2 + 27k^4)
\]

which has only one real root at \( k = 0 \). Substituting at \( k = \pm 1 \) we get \( D_{j_4,k}(-1) = D_{j_4,k}(1) = -382648320 < 0 \). Therefore \( D_{j_4,k}(k) \leq 0 \) \( \forall k \in I \) and \( j_4'(k, m) \) exactly one real root. If \( k \in I \) this root is not in \( \Omega \) since \( j_4'(k, 1) = -384k^2 - 256 < 0 \) \( \forall k, \) and \( j_4'(k, 2) = 441k^4 - 1344k^2 - 1024 < 0 \) \( \forall k \in I \). Same argument as before is valid to conclude \( \frac{\partial f}{\partial x_5}(x^*(k, m)) \) is negative in our domain.

b) Suppose \( \hat{x} \geq 1 \):

The function \( \frac{\partial f}{\partial x_5} \bigg|_1 = -6(9k^2 + 6k + 1)m + 96 \) is negative if and only if \( m > \frac{16}{9k^2 - 6k + 1} \).

The value \( m^* \) defined in Lemma A.4 is grater than \( \frac{16}{9k^2 - 6k + 1} \) for all \( k \in [-1/3, 1] \). Hence \( \frac{\partial f}{\partial x_2} \bigg|_1 \) is negative for all \( m > m^* \).

Lemma A.8. \( \frac{\partial f_{1324}}{\partial x_5} \bigg|_{x^*} \) is negative for all \( (k, m) \in I \times \Omega \).
The two first possible values of $I_{\cap}$ as $(14)$

$$\partial f_{1,3,24} \bigg|_{x^*} = 48\tilde{x}^4 + (-36k^2m - 12k^2 + 48)\tilde{x}^2 + (-36km - 12k)\tilde{x}$$

Let $p(x, k, m) = 48x^4 + (-36k^2m - 12k^2 + 48)x^2 + (-36km - 12k)x$ and $I = (p(x, k, m), p_\alpha(x, g, a, k, m))$. In this case the ideal defined as $I \cap \mathbb{C}[k,m]$ is generated by the polynomial

$$j(k, m) = k^4(m - 1)(3m + 1)^3(9k^2m + 3k^2 - 4)^3.$$ 

This polynomial vanishes if and only if $m = 1$, $m = -1/3$, $m = \frac{4 - 3k^2}{9k^2}$ or $k = 0$. The two first possible values of $m$ do not belong to $\Omega$. The third one does not satisfy $p(x, k, m) = 0$. It only remains to study the case $k = 0$ which is in $\mathcal{V}(I)$ for all values of $m$. However $\frac{\partial f_{1,3,24}}{\partial x_5} \bigg|_{x^*} has a unique root in $I \times \Omega$ and for random values of $k$ and $m$ at this region (for both $k$ positive and negative) we check that it is always negative.

b) Suppose $\tilde{x} \geq 1$:

The function $\frac{\partial f_{1,3,24}}{\partial x_5} |_1 = -6(9k^2 + 6k + 1)m + 96$ is negative if and only if $m > \frac{16}{9k^2 - 6k + 1}$. The value $m^*$ obtained in Lemma A.4 is greater than $m > \frac{16}{9k^2 - 6k + 1}$ for all $k \in [-1/3, 1]$. Thus $\frac{\partial f_{1,3,24}}{\partial x_2} |_1$ is negative for all $m > m^*$.

\[ \square \]

**Lemma A.9.** Let $g(x_1, x_3) = f(x_1, 1, x_3, 1, 1)$. Then $\tilde{x} = (\tilde{x}(k, m), \tilde{x}(k, m))$ is a minimum of $g$.

**Proof.** a) Assume $\tilde{x} \leq 1$

The first derivatives of $g(x_1, x_3)$ vanish at the point $\bar{x} = (\kappa(k, m), \kappa(k, m))$. The Hessian matrix of $g$ evaluated at $\bar{x}$ is,

$$H = \begin{pmatrix}
72\tilde{x}(k, m)^2 + 24 & -54k^2m - 18k^2 + 144\tilde{x}(k, m)^2 \\
-54k^2m - 18k^2 + 144\tilde{x}(k, m)^2 & 72\tilde{x}(k, m)^2 + 24
\end{pmatrix}$$

We need to prove that $H$ is a positive definite matrix, and therefore that all its principal minors are positive for all $k \in I$ and $m \in \Omega$. The first one is clearly positive since it is the sum of positive numbers. To prove that the determinant of $H$ is also positive we will follow the same ideas of Lemma A.5. Consider the ideal $\mathcal{I} = (\det(M), p_\alpha(x, g, a, k, m))$ where

$$\det(M) = 36(-9(3k^2m + k^2 - 8x^2)^2 + 16(3x^2 + 1)^2).$$

The elimination ideal $\mathcal{I} \cap \mathbb{C}[k, m] is generated by the polynomial $j(k, m) = j_1(k, m)j_2(k, m)j_3(k, m)$ where
\[ j_1 = 729k^6m^3 + 729k^6m^2 + 243k^6m + 27k^6 - 972k^4m^2 - 648k^4m - 108k^4 + 432k^2m + 144k^2 - 64, \]
\[ j_2 = 27k^2m^2 - 126k^2m - 45k^2 - 64 \text{ and } \]
\[ j_3 = 729k^6m^3 + 729k^6m^2 + 243k^6m + 27k^6 - 972k^4m^2 - 648k^4m - 108k^4 - 729k^2m^2 - 54k^2m + 63k^2 - 64. \]

We are interested in the zeros of each polynomial \( j_i \). The first one, \( j_1(k, m) \) only vanishes if \( m = \frac{4 - 3k^2}{9k^2} \) but this value is not a zero of \( \det(M) \). The polynomial \( j_2(k, m) \) vanishes at \( m = \frac{21k \pm 8\sqrt{9k^2 + 3}}{9k} \notin \Omega \) for any \( k \in I \). Consider \( j_{3,k}(m) = j_3(k, m) \) as a function of \( m \). Its discriminant \( D(k) = -297538935552k^8 - 99179645184k^6 \) is negative for all \( k \neq 0 \). Since \( j_{3,0}(m) = -64 \) for all \( m \), the polynomial \( j_{3,k}(m) \) has at most one real root \( \forall k \). Moreover, \( j_{3,k}(1) \leq 0 \) and \( j_{3,k}(\omega) \leq 0 \) for all \( k \) and hence \( j_{3,k} \) is smaller or equal than zero for all \( m \in \Omega \).

Therefore it can be deduced that \( \det(M) \) has constant sign in the region \( I \times \Omega \). Substituting at any random point on that region we can check that \( \det(M) > 0 \) for all \( k \in I \) and \( m \in \Omega \). And hence \( H \) is a positive definite matrix for all \( k \in I \) and \( m \in \Omega \).

\( b) \) Assume \( \tilde{x} \geq 1 \). In this case, since we are in the boundary of the domain, by the KKT conditions we need to prove that \( \nabla g(1, 1) \) is negative. The gradient

\[ \nabla g(1, 1) = (-54k^2m - 18k^2 - 18km - 6k + 96, -54k^2m - 18k^2 - 18km - 6k + 96) \]

is zero if and only if \( m = m^\ast \). Moreover for \( m \geq m^\ast \) or equivalently for \( \tilde{x} \geq 1 \) the polynomial \(-54k^2m - 18k^2 - 18km - 6k + 96 \) is negative for all \( k \in I \). 

\( \square \)