

THE EMBEDDING PROBLEM FOR MARKOV MATRICES

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Abstract: Characterizing whether a Markov process of discrete random variables has a homogeneous continuous-time realization is a hard problem. In practice, this problem reduces to deciding when a given Markov matrix can be written as the exponential of some rate matrix (a Markov generator). This is an old question known in the literature as the *embedding problem* [11], which has been solved only for matrices of size 2×2 or 3×3 . In this paper, we address this problem and related questions and obtain results along two different lines. First, for matrices of any size, we give a bound on the number of Markov generators in terms of the spectrum of the Markov matrix. Based on this, we establish a criterion for deciding whether a generic (distinct eigenvalues) Markov matrix is embeddable and propose an algorithm that lists all its Markov generators. Then, motivated and inspired by recent results on substitution models of DNA, we focus on the 4×4 case and completely solve the embedding problem for any Markov matrix. The solution in this case is more concise as the embeddability is given in terms of a single condition.

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1. Introduction

Markov matrices are used to describe changes between the states of two discrete random variables in a Markov process. As the entries of Markov matrices (or transition matrices) represent the conditional probabilities of substitution between states, Markov matrices have non-negative entries and rows summing to 1. Among them, embeddable matrices are those that are consistent with a homogeneous continuous-time Markov process, so that changes occur at a constant rate over time and time is conceived as a continuous concept. The instantaneous rates of substitution are usually displayed as the entries of real matrices with non-negative off-diagonal entries and rows summing to 0, so-called *rate matrices*. In the homogeneous continuous-time setting, the transition matrices of a Markov process can be computed as $M(t) = e^{Qt}$, where Q is the rate matrix ruling the process and $t \geq 0$ accounts for the time

elapsed in the process. In this case, M is said to be *embeddable*. Equivalently, a Markov matrix M is embeddable if it can be written as the exponential of a rate matrix Q , $M = e^Q$ (with no reference to time t). Any rate matrix Q satisfying $M = e^Q$ is called a *Markov generator* of M .

Almost a century ago, Elfving ([11]) formulated the problem of deciding which Markov matrices are embeddable, *the embedding problem*. Solving the embedding problem results in giving necessary and sufficient conditions for a Markov matrix M to be the exponential of a rate matrix Q , $M = e^Q$. Although the question is quite theoretical, it has practical consequences and, as such, it may appear in any applied field where discrete and continuous-time Markov processes are considered. For instance, in economic sciences [20, 15], in social sciences [29], and in evolutionary biology [32, 21], the embedding problem is crucial for deciding whether a Markov process can be modeled as a homogeneous continuous-time process or not.

Although the embedding problem is solved for 2×2 and 3×3 matrices [24, 10, 22, 4], it has remained open for larger matrices so far. Some partial results on the necessary conditions for a Markov matrix to be embeddable were given in the second part of the twentieth century [28, 24, 9]. Moreover, there exist sufficient and necessary conditions on the embeddability of Markov matrices with *different and real* eigenvalues. This is a consequence of a result due to Culver [8] and characterizes embeddability of this type of matrices in terms of the principal logarithm; see Corollary 2.8. There are also some inequalities that need to be satisfied by the determinant or the entries of the matrix in order to be embeddable [16, 13]. At the same time, there is a discrete version of the embedding problem, which consists in deciding when a Markov matrix can be written as a certain power of another Markov matrix (see [29, 17, 18] for instance).

A related issue is that of deciding whether there is a unique Markov generator for a given embeddable Markov matrix. Note that each Markov generator provides a different embedding of the Markov matrix into a homogeneous continuous-time Markov process. We refer to this question as the *rate identifiability problem*. It is well known that for diagonally dominant embeddable matrices the number of Markov generators reduces to one [9, Theorem 4]. The same happens if the matrix is close to the identity; for example, if either $\|M - I\| < 0.5$ or $\det(M) > 0.5$ [20]. However, the situation becomes really complicated as the determinant of the matrix decreases. The first example of a Markov matrix with more than one Markov generator was given in [30], and further examples were provided in [10, 20]. In all these examples, however, the principal logarithm happens to be a rate matrix.

In this paper we provide a solution to the embedding problem for Markov matrices of any size with pairwise *different* eigenvalues (not necessarily real); see Theorem 4.5. This situation covers a dense open subset of the space of Markov matrices, so it solves the embedding problem almost completely (the set of matrices with repeated eigenvalues has measure zero within the whole space of matrices). For such matrices, we bound the number of Markov generators in terms of the real and imaginary parts of the eigenvalues and establish a criterion for deciding whether a Markov matrix with different eigenvalues is embeddable. Based on this criterion, we provide an algorithm that gives *all* Markov generators for Markov matrices with different eigenvalues (Algorithm 4.7). We also give an improvement in the bounds on the determinant mentioned above; see Corollary 3.3. The main techniques are the description of the complex logarithms of a matrix (see [14]) and a careful study of the complex region where the eigenvalues of a rate matrix lie (Section 3).

In addition to these results, we completely solve the embedding problem for 4×4 Markov matrices (with *repeated or different* eigenvalues). The solution to the embedding problem provided in this case (see Section 5) is much more satisfactory because we are able to characterize embeddability by checking a single condition (and not looking at a list of possible Markov generators). We have devoted special attention to 4×4 matrices not only because it was the first case that remained still open, but also because our original approach and motivation arises from the field of phylogenetics, where Markov matrices rule the substitution of nucleotides in the evolution of DNA molecules. In recent years, new results and advances concerning the embedding problem have appeared in this field, providing deep insight and illustrative examples of the complexity of the general situation; see [21, 27, 1, 5]. The present work builds on some previous contributions by the authors in this setting.

For 4×4 Markov matrices M with different eigenvalues (real or not) we prove that the embeddability can be checked directly by looking at the principal logarithm $\text{Log}(M)$ together with a basis of eigenvectors:

Theorem 1.1. *Let $M = P \text{diag}(1, \lambda_1, \lambda_2, \lambda_3) P^{-1}$ be a 4×4 Markov matrix with $\lambda_1 \in \mathbb{R}_{>0}$, $\lambda_2 \in \mathbb{C}$, $\lambda_3 \in \mathbb{C}$ pairwise different. If $\lambda_2, \lambda_3 \notin \mathbb{R}$, define $V = P \text{diag}(0, 0, 2\pi i, -2\pi i) P^{-1}$,*

$$\mathcal{L} := \max_{(i,j): i \neq j, V_{i,j} > 0} \left[-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \right], \quad \mathcal{U} := \min_{(i,j): i \neq j, V_{i,j} < 0} \left[-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \right],$$

and define $V = 0$, $\mathcal{L} = \mathcal{U} = 0$ if all eigenvalues are real. Set

$$\mathcal{N} := \{(i, j) : i \neq j, V_{i,j} = 0, \text{ and } \text{Log}(M)_{i,j} < 0\}.$$

Then, M is embeddable if and only if $\mathcal{N} = \emptyset$, $\mathcal{L} \leq \mathcal{U}$, and $\lambda_i \notin \mathbb{R}_{\leq 0}$ for $i = 1, 2, 3$. In this case, the Markov generators of M are the matrices $\text{Log}(M) + kV$, where $k \in \mathbb{Z}$ satisfies $\mathcal{L} \leq k \leq \mathcal{U}$.

As a byproduct we give an algorithm that outputs *all* possible Markov generators for such a matrix. Apart from this general case of matrices with different eigenvalues, we also study all other cases within the 4×4 case and we give an embeddability criterion for each (see Subsection 5.1, Cases I, II, III, IV, and Subsection 5.2). The case of diagonalizable matrices with *two* real repeated eigenvalues (Case III) turns out to be much more involved; still we are able to provide necessary and sufficient conditions for the embeddability in terms of eigenvalues and eigenvectors, and to propose an algorithm that checks whether a Markov matrix in this case is embeddable (Corollary 5.14, Algorithm 5.16).

The outline of the paper is as follows. In Section 2 we state with precision the embedding problem and recall some known results needed in the sequel. Section 3 is devoted to bounding the real and the imaginary part of the eigenvalues of any rate matrix (Lemma 3.1). These bounds are used in Section 4 in order to provide a sufficient and necessary condition for an $n \times n$ Markov matrix with pairwise different eigenvalues to be embeddable. In the same section, we also give the algorithm that outputs all Markov generators of such matrices. We devote Section 5 to 4×4 matrices, studying their embeddability in full detail by splitting them into all possible Jordan canonical forms. The proof of Theorem 1.1 is also given there. In the last section of the paper, Section 6, we summarize the results on the rate identifiability for embeddable 4×4 matrices (see Table 2). Appendix A is devoted to details concerning the implementation of Algorithm 5.16.

2. Preliminaries

In this section we recall some definitions and relevant facts about the embedding problem of Markov matrices.

Definition 2.1. A real square matrix M is a *Markov matrix* if its entries are non-negative and all its rows sum to 1. A real square matrix Q is a *rate matrix* if its off-diagonal entries are non-negative and its rows sum to 0. A Markov matrix M is *embeddable* if there is a rate matrix Q such that $M = e^Q$; in this case we say that Q is a *Markov generator* for M . Embeddable Markov matrices are also sometimes referred to as matrices that have a *continuous realization* [31]. The *embedding problem* ([11]) consists in deciding whether a given Markov matrix is embeddable or not, in other words, determining which Markov matrices can be embedded into the multiplicative semigroup $(\{e^{Qt} : t \geq 0\}, \cdot)$ for some rate matrix Q .

The following notation will be used throughout the paper. Id denotes the identity matrix of order n . We write $GL_n(\mathbb{K})$ for the space of $n \times n$ invertible matrices with entries in $\mathbb{K} = \mathbb{R}$ or \mathbb{C} . For $\lambda \in \mathbb{C} \setminus \{0\}$, we use the notation $\log_k(\lambda)$ to denote the k -th branch of the logarithm of λ , that is, $\log_k(\lambda) = \log|\lambda| + (\text{Arg}(\lambda) + 2\pi k)i$, where $\text{Arg}(\lambda) \in (-\pi, \pi]$ is the *principal argument* of λ . For ease of reading the principal logarithm $\log_0(\lambda)$ will be denoted as $\log(\lambda)$. Given a square matrix M , we denote by $\sigma(M)$ the set of all its eigenvalues and by $\text{Comm}^*(M)$ the *commutant* of M , that is, the set of invertible complex matrices that commute with M .

Remark 2.2. If D is a diagonal matrix,

$$D = \text{diag} \left(\overbrace{\lambda_1, \dots, \lambda_1}^{m_1}, \overbrace{\lambda_2, \dots, \lambda_2}^{m_2}, \dots, \overbrace{\lambda_l, \dots, \lambda_l}^{m_l} \right)$$

with $\lambda_i \neq \lambda_j$, then $\text{Comm}^*(D)$ consists of all the block-diagonal matrices whose blocks are taken from the corresponding $GL_{m_i}(\mathbb{C})$. In particular, the commutant of D does not depend on the particular values of the entries λ_i . If $m_1 = m_2 = \dots = m_l = 1$, then $\text{Comm}^*(D)$ is the set of invertible diagonal matrices.

If M is diagonalizable, the following result describes all possible *logarithms* of M (that is, all the solutions Q to the equation $M = e^Q$).

Theorem 2.3 ([14, §VIII.8]). *Given a non-singular matrix M with an eigendecomposition $P \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) P^{-1}$, where $\lambda_i \in \mathbb{C}$, $i = 1, \dots, n$, and $P \in GL_n(\mathbb{C})$, the following are equivalent:*

- (i) Q is a solution to the equation $M = e^Q$,
- (ii) $Q = P A \text{diag}(\log_{k_1}(\lambda_1), \log_{k_2}(\lambda_2), \dots, \log_{k_n}(\lambda_n)) A^{-1} P^{-1}$ for some $k_1, k_2, \dots, k_n \in \mathbb{Z}$ and some $A \in \text{Comm}^*(\text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n))$.

Remark 2.4. With respect to the previous result, we want to point out the following.

- (i) If u is an eigenvector of Q with eigenvalue a , then u is also an eigenvector of $M = e^Q$ with eigenvalue e^a . The converse is not true in general.
- (ii) If $\text{Comm}^*(\text{diag}(\lambda_1, \dots, \lambda_n)) = \text{Comm}^*(\text{diag}(\log_{k_1}(\lambda_1), \dots, \log_{k_n}(\lambda_n)))$, then the description of the logarithms is slightly simpler, as every logarithm can be written as

$$Q = P \text{diag}(\log_{k_1}(\lambda_1), \dots, \log_{k_n}(\lambda_n)) P^{-1}.$$

Moreover, in this case, M and Q have the same eigenvectors. This occurs, for example, when all the eigenvalues of M are pairwise distinct or also when $k_1 = k_2 = \dots = k_n$.

The well-known formula $\det e^Q = e^{\operatorname{tr} Q}$ implies that the determinant of every embeddable matrix is a positive real number. Hence, throughout this paper we implicitly assume that *all Markov matrices are non-singular and have a positive determinant*. Note that this is not a restriction of the original problem, but a necessary condition for a Markov matrix to be embeddable.

Since both Markov and rate matrices have only real entries, the study about the existence of real logarithms of real matrices by [8] is relevant for solving the embedding problem. The following proposition is a direct consequence of that work.

Proposition 2.5 (see [8, Theorem 1]). *Let M be a real square matrix. Then, there exists a real logarithm of M if and only if $\det(M) > 0$ and each Jordan block of M associated with a negative eigenvalue occurs an even number of times.*

In [8, Theorem 2], Culver also proved that matrices with pairwise distinct positive eigenvalues have only one real logarithm, namely, the *principal logarithm*:

Definition 2.6. The *principal logarithm* of M , which will be denoted by $\operatorname{Log}(M)$, is the only logarithm whose eigenvalues are the principal logarithm of the eigenvalues of M (see [19, Theorem 1.31]). In particular, if M is diagonalizable, then

$$\operatorname{Log}(M) = P \operatorname{diag}(\log(\lambda_1), \dots, \log(\lambda_n)) P^{-1}.$$

If M is a Markov matrix, then its principal logarithm $\operatorname{Log}(M)$ has row sums equal to 0 (although it may not be a real matrix).

Remark 2.7. Note that the above definition of the principal logarithm (Definition 2.6) extends the usual definition (e.g. see [19, p. 20]), which requires that the matrix M has no negative eigenvalues. This is required in order to use the spectral resolution of the logarithm function. In this paper, however, we mainly deal with diagonalizable matrices, for which the principal logarithm can be defined directly by taking the principal argument of the eigenvalues. The only non-diagonalizable Markov matrices that we deal with are 4×4 (see Subsection 5.2) which, according to Proposition 2.5, have no negative eigenvalues if they have a real logarithm.

As a byproduct of the results explained above, we get the following embeddability criterion for Markov matrices with pairwise distinct real eigenvalues in terms of its principal logarithm.

Corollary 2.8. *Let M be a Markov matrix with pairwise distinct real eigenvalues. Then:*

- (i) *If M has a non-positive eigenvalue, then M is not embeddable.*
- (ii) *If M has no negative eigenvalues, M is embeddable if and only if $\text{Log}(M)$ is a rate matrix.*

3. Bounds on the eigenvalues of rate matrices

It is well known that the eigenvalues of a Markov matrix have modulus smaller than or equal to 1 [25, §8.4]. Here we bound the real and the imaginary part of the complex eigenvalues of rate matrices. To this end, if Q is an $n \times n$ rate matrix with $n \geq 3$ and $\lambda \in \sigma(Q)$ is a non-real eigenvalue, we define

$$b_n(\lambda) := \min \left\{ \sqrt{2 \operatorname{tr}(Q) \operatorname{Re}(\lambda) - (\operatorname{Re}(\lambda))^2}, -\frac{\operatorname{Re}(\lambda)}{\tan(\pi/n)} \right\},$$

$$B_n := \min \left\{ -\frac{\sqrt{3}}{2} \operatorname{tr}(Q), -\frac{\operatorname{tr}(Q)}{2 \tan(\pi/n)} \right\}.$$

The following technical result is used in the next section and is also useful to improve a result of [20] (see Corollary 3.3).

Lemma 3.1. *Let Q be an $n \times n$ rate matrix. Then for any eigenvalue $\lambda \in \sigma(Q)$ we have*

- (i) $\operatorname{Re}(\lambda) \leq 0$. Moreover, if $\lambda \notin \mathbb{R}$, then $\frac{\operatorname{tr}(Q)}{2} \leq \operatorname{Re}(\lambda) \leq 0$.
- (ii) $|\operatorname{Im}(\lambda)| \leq b_n(\lambda) \leq B_n$ if $\lambda \notin \mathbb{R}$.

Moreover, the bound on $|\operatorname{Im}(\lambda)|$ given by $b_n(\lambda)$ is tight for $n \geq 3$.

Proof: (i) If Q is a rate matrix, then e^Q is a Markov matrix. In particular, the eigenvalues of Q are logarithms of the eigenvalues of a Markov matrix. Since the modulus of the eigenvalues of a Markov matrix is bounded by 1, we get $\operatorname{Re}(\lambda) \leq 0$ for any $\lambda \in \sigma(Q)$. Moreover, as non-real eigenvalues of Q appear in conjugate pairs, we have that

$$\operatorname{tr}(Q) = \sum_{\lambda \in \sigma(Q)} \lambda = \sum_{\lambda \in \sigma(Q) \cap \mathbb{R}} \lambda + \sum_{\lambda \in \sigma(Q) \setminus \mathbb{R}} \operatorname{Re}(\lambda).$$

Therefore, if $\lambda \notin \mathbb{R}$, then $\operatorname{Re}(\lambda)$ appears twice in this expression, and so $\operatorname{Re}(\lambda) \geq \operatorname{tr}(Q)/2$.

- (ii) We prove first that, for any non-real eigenvalue $\lambda \in \sigma(Q)$, we have

$$(1) \quad |\operatorname{Im}(\lambda)| \leq \sqrt{2 \operatorname{tr}(Q) \operatorname{Re}(\lambda) - (\operatorname{Re}(\lambda))^2} \leq -\frac{\sqrt{3}}{2} \operatorname{tr}(Q).$$

Let us take $r = -\operatorname{tr}(Q)$. Since Q is a rate matrix we get that $\tilde{Q} = Q + r\operatorname{Id}_n$ is a matrix with non-negative entries whose rows sum to r . Then any eigenvalue $\tilde{\lambda} \in \sigma(\tilde{Q})$ has modulus smaller than or equal to r (see [25, §8.3]). Now, if λ is an eigenvalue of Q , we have that $\lambda + r \in \sigma(\tilde{Q})$. Therefore, $(\operatorname{Re}(\lambda) + r)^2 + \operatorname{Im}(\lambda)^2 = |\lambda + r|^2 \leq r^2$ and we obtain

$$(2) \quad |\operatorname{Im}(\lambda)| \leq \sqrt{r^2 - (\operatorname{Re}(\lambda) + r)^2} = \sqrt{2\operatorname{Re}(\lambda)\operatorname{tr}(Q) - \operatorname{Re}(\lambda)^2}.$$

The second inequality in (1) follows by using $0 \geq \operatorname{Re}(\lambda) \geq \operatorname{tr}(Q)/2$ in (2).

We prove now that

$$(3) \quad |\operatorname{Im}(\lambda)| \leq -\frac{\operatorname{Re}(\lambda)}{\tan(\pi/n)} \leq -\frac{\operatorname{tr}(Q)}{2\tan(\pi/n)}$$

for any non-real eigenvalue λ of Q . If $n < 3$, then Q has no complex eigenvalue, because 0 is an eigenvalue of any rate matrix and complex eigenvalues of real matrices appear in conjugate pairs. If $n \geq 3$, the first theorem in [28] claims that the principal argument of any eigenvalue $\lambda \in \sigma(Q)$ is bounded as

$$(4) \quad \left(\frac{1}{2} + \frac{1}{n}\right)\pi \leq |\operatorname{Arg}(\lambda)|.$$

Then the first inequality in (3) is obtained by using that $\operatorname{Im}(\lambda) = \tan(\operatorname{Arg}(\lambda))\operatorname{Re}(\lambda)$, $\operatorname{Re}(\lambda) \leq 0$, and that $|\tan|$ restricted to $(-\pi, -\pi/2 - \pi/n] \cup [\pi/2 + \pi/n, \pi]$ attains its maximum at

$$(5) \quad \left|\tan\left(-\frac{\pi}{2} - \frac{\pi}{n}\right)\right| = \left|\tan\left(\frac{\pi}{2} + \frac{\pi}{n}\right)\right| = \frac{1}{\tan(\pi/n)} > 0.$$

The second inequality follows by using $\operatorname{Re}(\lambda) \geq \operatorname{tr}(Q)/2$.

From the first inequality in both (1) and (3), we have $|\operatorname{Im}(\lambda)| \leq b_n(\lambda)$. On the other hand, the inequality $b_n(\lambda) \leq B_n$ follows from the definition of $b_n(\lambda)$ and the second inequalities in (1) and (3). This concludes the proof of (ii).

Next, we show that the bound on $|\operatorname{Im}(\lambda)|$ given by $b_n(\lambda)$ is tight for $n \geq 3$. As shown in [28, Theorem on p. 537], for each $n \geq 3$, there is an $n \times n$ rate matrix Q with at least one eigenvalue satisfying (4) with equality. Such a matrix is given by

$$q_{ij} = \begin{cases} -\alpha & \text{if } i = j, \\ \alpha & \text{if } i \equiv j - 1 \pmod{n}, \\ 0 & \text{otherwise,} \end{cases}$$

where α is an arbitrary positive number. It can be seen that this matrix Q has at least a non-real eigenvalue λ satisfying $|\operatorname{Im}(\lambda)| = \left|\operatorname{Re}(\lambda)\tan\left(\frac{\pi}{2} + \frac{\pi}{n}\right)\right|$. Using that $\operatorname{Re}(\lambda) < 0$ together with (5), we get $-\frac{\operatorname{Re}(\lambda)}{\tan(\pi/n)} =$

$|\text{Im}(\lambda)| \leq b_n(\lambda)$. The definition of $b_n(\lambda)$ implies that $|\text{Im}(\lambda)| = b_n(\lambda)$, so the inequality is tight. \square

Remark 3.2. Note that for $n \geq 2$ we have $\tan(\pi/n) > \tan(\pi/(n + 1))$. As for $n = 6$ $\tan(\pi/n)$ is $1/\sqrt{3}$, we obtain that

$$B_n = \begin{cases} -\frac{\text{tr}(Q)}{2 \tan(\pi/n)} & \text{if } n = 3, 4, 5, 6, \\ -\frac{\sqrt{3}}{2} \text{tr}(Q) & \text{if } n \geq 6. \end{cases}$$

Although for $n > 6$ the value in the minimum defining $b_n(\lambda)$ depends on λ , for $n \leq 6$ we have $b_n(\lambda) = -\frac{\text{Re}(\lambda)}{\tan(\pi/n)}$. Indeed, if $n \in \{3, 4, 5, 6\}$, then

$$\begin{aligned} -\frac{\text{Re}(\lambda)}{\tan(\pi/n)} &\leq -\text{Re}(\lambda)\sqrt{3} \\ &= \sqrt{4\text{Re}(\lambda)^2 - \text{Re}(\lambda)^2} \leq \sqrt{2 \text{tr}(Q) \text{Re}(\lambda) - (\text{Re}(\lambda))^2}. \end{aligned}$$

Figure 1 illustrates both the remark above and Lemma 3.1.

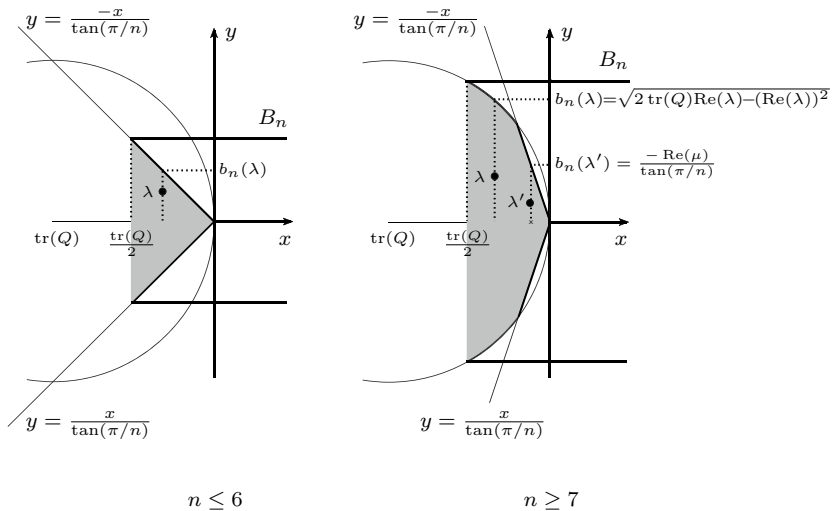


FIGURE 1. The shaded area is the complex region containing the eigenvalues of $n \times n$ rate matrices (Lemma 3.1) according to the two cases described in Remark 3.2. For $n \leq 6$, we have that $B_n = -\frac{\text{tr}(Q)}{2 \tan(\pi/n)}$ and $b_n(\lambda) = -\frac{\text{Re}(\lambda)}{\tan(\pi/n)}$, while for $n \geq 7$, $B_n = -\frac{\sqrt{3}}{2} \text{tr}(Q)$ and the expression for $b_n(\lambda)$ depends on the value of λ as illustrated by the eigenvalues λ and λ' in the figure. All these bounds are represented in black in the figure.

The following result improves the bound given in [20, Theorem 5.1], which states that a Markov matrix M with pairwise distinct eigenvalues and $\det(M) > e^{-\pi}$ is embeddable if and only if $\text{Log}(M)$ is a rate matrix. We are able to relax the hypothesis on the determinant and avoid the condition of distinct eigenvalues.

Corollary 3.3. *Let M be an $n \times n$ Markov matrix with $\det(M) > \min\{e^{-\frac{2\pi}{\sqrt{3}}}, e^{-2\pi \tan(\pi/n)}\}$. Then, the only possible Markov generator for M is $\text{Log}(M)$. In particular, M is embeddable if and only if $\text{Log}(M)$ is a rate matrix.*

Proof: Let Q be a Markov generator for M . By hypothesis, $\text{tr}(Q) = \log(\det(M))$ is strictly greater than $\min\{-\frac{2\pi}{\sqrt{3}}, -2\pi \tan(\pi/n)\}$. Therefore, using Lemma 3.1(ii), we have $|\text{Im}(\lambda)| \leq B_n < \pi$ for all $\lambda \in \sigma(Q)$. Hence, Q is the principal logarithm of M . \square

Remark 3.4. As in Remark 3.2, we have that $e^{-2\pi \tan(\pi/n)} \leq e^{-\frac{2\pi}{\sqrt{3}}}$ for $n = 3, 4, 5, 6$ and $e^{-2\pi \tan(\pi/n)} \geq e^{-\frac{2\pi}{\sqrt{3}}}$ for $n \geq 6$.

Table 1 gives numerical values for the bound in Corollary 3.3.

Size of M	$n = 3$	$n = 4$	$n = 5$	$n \geq 6$
Bound on $\det(M)$	0.000019	0.001867	0.010410	0.026580

TABLE 1. Lower bounds on the determinant (rounded to the 6th decimal) that allow the characterization of the embeddability in terms of the principal logarithm of an $n \times n$ Markov matrix according to Corollary 3.3 and Remark 3.4. Previously known bounds were $e^{-\pi} = 0.043214$ and 0.5 for all $n \in \mathbb{N}$ (see [10] and [20], respectively), which have been improved by Corollary 3.3.

4. Embeddability of Markov matrices with (non-real) distinct eigenvalues

In this section we deal with Markov matrices with pairwise distinct eigenvalues. It is known that the embeddability of these matrices is determined by the principal logarithm if all the eigenvalues are *real* (see Corollary 2.8). However, this may not be the case if there is a non-real eigenvalue [26]. By virtue of Proposition 2.5, we know that every (real) matrix M with distinct eigenvalues has some real logarithm; by [8, Theorem 2 and Corollary], we also know that if M has complex eigenvalues, then there are countably-infinitely many logarithms. In this section, we

give a precise description of those real logarithms with rows summing to 0 (Proposition 4.3) and we show that only a finite subset of them have non-negative off-diagonal entries (Theorem 4.5). In this way we are able to design an algorithm that returns the Markov generators of a Markov matrix with distinct eigenvalues (real or not); see Algorithm 4.7.

As pointed out in the preliminaries section, it is well known that a necessary condition for a Markov matrix to be embeddable is to have a positive determinant. If we assume that all eigenvalues are distinct, then this implies that the real eigenvalues lie in the interval $(0, 1]$. Throughout this section we consider matrices satisfying the following assumption:

Assumption 4.1. *We assume that M is a (non-singular) diagonalizable $n \times n$ Markov matrix with pairwise distinct eigenvalues and whose real eigenvalues lie in the interval $(0, 1]$. Without loss of generality, we can write*

$$M = P \operatorname{diag}(1, \lambda_1, \dots, \lambda_t, \mu_1, \overline{\mu_1}, \dots, \mu_s, \overline{\mu_s}) P^{-1}$$

for some $P \in GL_n(\mathbb{C})$, $\lambda_i \in (0, 1)$ with $i = 1, \dots, t$, and $\mu_j \in \{z \in \mathbb{C} : \operatorname{Im}(z) > 0\}$ with $j = 1, \dots, s$, all of them pairwise distinct.

Definition 4.2. Given a Markov matrix M as in Assumption 4.1, for each $(k_1, \dots, k_s) \in \mathbb{Z}^s$ we define the following matrix:

$$\begin{aligned} \operatorname{Log}_{k_1, \dots, k_s}(M) := & P \operatorname{diag}(0, \log(\lambda_1), \dots, \log(\lambda_t), \log_{k_1}(\mu_1), \overline{\log_{k_1}(\mu_1)}, \dots \\ & \dots, \log_{k_s}(\mu_s), \overline{\log_{k_s}(\mu_s)}) P^{-1}. \end{aligned}$$

Note that $\operatorname{Log}_{0, \dots, 0}(M)$ is the principal logarithm of M , $\operatorname{Log}(M)$.

The next result claims that these are all the real logarithms of the matrix M .

Proposition 4.3. *Let M be a Markov matrix as in Assumption 4.1. Then, a matrix Q with rows summing to 0 is a real logarithm of M if and only if $Q = \operatorname{Log}_{k_1, \dots, k_s}(M)$ for some $k_1, \dots, k_s \in \mathbb{Z}$.*

Proof: We know that the first column of P is an eigenvector of M with eigenvalue 1. Since the rows of M sum to 1 and it has no repeated eigenvalue we can assume without loss of generality that it is the eigenvector $(1, 1, \dots, 1)$. In addition, we know that for $m = 1, \dots, s$ the $(t + 2m)$ -th and $(t + 2m + 1)$ -th columns of P can be chosen to be conjugates because M is real.

⇐) Using that $\overline{\log_k(\mu)} = \log_{-k}(\bar{\mu})$ it follows from Theorem 2.3 that $\text{Log}_{k_1, \dots, k_s}(M)$ is a logarithm of M for any $k_1, \dots, k_s \in \mathbb{Z}$. Note that the rows of Q sum to 0 because the first column of P is the eigenvector $(1, 1, \dots, 1)$ and its corresponding eigenvalue is 0. Moreover, the non-real eigenvalues of Q appear in conjugate pairs and the corresponding eigenvectors appearing as column vectors in P are also a conjugate pair, thus Q is real.

⇒) Let Q be a real logarithm of M with rows summing to 0. Since M has pairwise distinct eigenvalues so does Q . Moreover, Q is diagonalizable through P (see Remark 2.4(ii)). Hence, it follows from Theorem 2.3 that:

$$Q = P \text{diag}(\log_{k_0}(1), \log_{k_1}(\lambda_1), \dots, \log_{k_t}(\lambda_t), \dots, \log_{k_{t+1}}(\mu_1), \log_{k_{t+2}}(\bar{\mu}_1), \dots, \log_{k_{t+2s-1}}(\mu_s), \log_{k_{t+2s}}(\bar{\mu}_s))P^{-1}.$$

Since the rows of Q sum to 0 we get that $k_0 = 0$. Since Q is real and has no repeated eigenvalues it follows that $k_1 = k_2 = \dots = k_t = 0$ and that its non-real eigenvalues appear in conjugate pairs. Hence, $\log_{k_{t+2m-1}}(\bar{\mu}_m) = \log_{k_{t+2m}}(\mu_m)$. \square

Remark 4.4. When all the eigenvalues of M are real (that is, $s = 0$), the proposition above claims that the only real logarithm with rows summing to 0 is the principal logarithm.

From the proposition above and Lemma 3.1 we get that any Markov matrix with pairwise distinct eigenvalues has a finite number of Markov generators. Hence, its embeddability can be determined by checking whether a finite family of well-defined matrices contains a rate matrix or not, as stated in the next result. In order to simplify the notation, for a given Markov matrix M and for any $z \in \mathbb{C}$ we define

$$\beta_n(z) := \min \left\{ \sqrt{2 \log(\det(M)) \log |z| - \log^2 |z|}, -\frac{\log |z|}{\tan(\pi/n)} \right\}.$$

If Q is a Markov generator of M and $\log_k(z)$ is an eigenvalue of Q , then $\beta_n(z) = b_n(\log_k(z))$. Hence, according to Lemma 3.1 we have $\beta_n(z) = -\frac{\log |z|}{\tan(\pi/n)}$ for $n = 3, 4, 5, 6$.

Theorem 4.5. *If M is a Markov matrix as in Assumption 4.1, then*

- (i) M is embeddable if and only if $\text{Log}_{k_1, \dots, k_s}(M)$ is a rate matrix for some $(k_1, \dots, k_s) \in \mathbb{Z}^s$ satisfying $\left\lceil \frac{-\text{Arg}(\mu_j) - \beta_n(\mu_j)}{2\pi} \right\rceil \leq k_j \leq \left\lfloor \frac{-\text{Arg}(\mu_j) + \beta_n(\mu_j)}{2\pi} \right\rfloor$ for $j = 1, \dots, s$.
- (ii) M has at most $\left\lfloor 1 - \frac{\sqrt{3} \log(\det(M))}{2\pi} \right\rfloor^s$ Markov generators if $n \geq 6$, at most $\left\lfloor 1 - \frac{\log(\det(M))}{2\pi \tan(\pi/n)} \right\rfloor^s$ if $n = 3, 4, 5$, and at most 1 if $n \leq 2$.

Proof: If Q is a logarithm of M , then $\log(\det(M)) = \text{tr}(Q)$. Hence, since $\text{Re}(\log_k(\mu)) = \log|\mu|$ we have that $\beta_n(\mu) = b_n(\log_k(\mu))$ for any $k \in \mathbb{Z}$ and any $\mu \in \sigma(M)$.

- (i) Let Q be a Markov generator for M . According to Proposition 4.3 there exist $k_1, \dots, k_s \in \mathbb{Z}$ such that $Q = \text{Log}_{k_1, \dots, k_s}(M)$. Now, by Lemma 3.1 we have $|\text{Im}(\log_{k_j}(\mu_j))| \leq \beta_n(\mu_j)$. We get the asserted bounds by using that $|\text{Im}(\log_{k_j}(\mu_j))| = |\text{Arg}(\mu_j) + 2\pi k_j|$.
- (ii) If $n < 3$, then M has only real eigenvalues and hence its only possible Markov generator is $\text{Log}(M)$. For other values of n , it follows from the first statement that if $\text{Log}_{k_1, \dots, k_s}(M)$ is a Markov generator, then k_j lies in an interval of length $\frac{2\beta_n(\mu_j)}{2\pi}$. Since $k_j \in \mathbb{Z}$ for all j we get that M has at most $\prod_j \left\lfloor 1 + \frac{2\beta_n(\mu_j)}{2\pi} \right\rfloor$ generators.

The statement follows by using Lemma 3.1 and Remark 3.2 to get

$$\beta_n(\mu) = \begin{cases} -d \frac{\log(\det(M))}{2 \tan(\pi/n)} & \text{if } n = 3, 4, 5, 6, \\ -\frac{\sqrt{3}}{2} \log(\det(M)) & \text{if } n \geq 6. \end{cases} \quad \square$$

Remark 4.6. As shown in the proof of Theorem 4.5(ii), the number of Markov generators of M is also bounded by $\prod_j \left\lfloor 1 + \frac{2\beta_n(\mu_j)}{2\pi} \right\rfloor$. Although this bound improves those in Theorem 4.5(ii), we do not know if it is sharp or not and we prefer to give a bound depending on $\log(\det(M))$ because this quantity might be related to the expected number of substitutions of the Markov process ruled by M (see [3] for further details on this in the context of phylogenetics).

To close this section, we present an algorithm which determines the embeddability of a Markov matrix with pairwise distinct eigenvalues and returns all its Markov generators.

Algorithm 4.7 (Markov generators for $n \times n$ matrices with distinct eigenvalues).

```

input :  $M$ , an  $n \times n$  Markov matrix with no repeated eigenvalues.
output: All its Markov generators if  $M$  is embeddable, an empty
         list otherwise.

generators=[ ]
compute eigenvalues of  $M$ 
if  $M$  has a negative or zero eigenvalue, then
  | return “ $M$  not embeddable”
  | exit
else
  |  $s = \frac{\#\text{non-real eigenvalues}}{2}$ 
  | if  $s > 0$  (i.e.  $M$  has a non-real eigenvalue), then
  |   | for  $j = 1, \dots, s$  do
  |     |  $\lfloor$  set  $l_j = \lfloor \frac{-\text{Arg}(\mu_j) - \beta_n(\mu_j)}{2\pi} \rfloor$  and  $u_j = \lfloor \frac{-\text{Arg}(\mu_j) + \beta_n(\mu_j)}{2\pi} \rfloor$ 
  |     | for  $k_1 = l_1, \dots, u_1$  do
  |       |  $\vdots$ 
  |       | for  $k_s = l_s, \dots, u_s$  do
  |         | compute  $\text{Log}_{k_1, \dots, k_s}(M)$ 
  |         | if  $\text{Log}_{k_1, \dots, k_s}(M)$  is a rate matrix, then
  |           |  $\lfloor$  add  $\text{Log}_{k_1, \dots, k_s}(M)$  to generators
  |         |
  |       |
  |     |
  |   |
  | else
  |   | if  $\text{Log}(M)$  is a rate matrix, then
  |     |  $\lfloor$  add  $\text{Log}(M)$  to generators
  |   |
  | if generators=[ ], then
  |   | return “ $M$  not embeddable”
  |   |
  | else
  |   | return generators
  |

```

Remark 4.8. As stated in Corollary 3.3, if M has a Markov generator other than $\text{Log}(M)$, then M has a small determinant and some eigenvalues of M are close to 0. In this case there might be numerical issues in the implementation of the algorithm.

5. Embeddability of 4×4 Markov matrices

In this section we study the embedding problem for all 4×4 Markov matrices. In this case, we can be more precise than in Theorem 4.5 and,

for matrices with distinct eigenvalues, we manage to give a criterion for the embeddability in terms of the eigenvectors; see Corollary 5.6. We are also able to deal with repeated eigenvalues so that the results of this section include all possible 4×4 Markov matrices.

5.1. Embeddability of diagonalizable 4×4 Markov matrices.

Using Proposition 2.5 and the fact that the modulus of the eigenvalues of a Markov matrix is bounded by 1, we are able to enumerate all possible diagonal forms of a diagonalizable 4×4 Markov matrix with real logarithms (up to ordering the eigenvalues):

Lemma 5.1. *Let M be a diagonalizable 4×4 Markov matrix. If M admits a real logarithm, then its diagonal form lies necessarily in one of the following cases (up to ordering the eigenvalues):*

- Case I $\text{diag}(1, \lambda_1, \lambda_2, \lambda_3)$ with $\lambda_1, \lambda_2, \lambda_3 \in (0, 1]$ pairwise distinct.
- Case II $\text{diag}(1, \lambda, \mu, \bar{\mu})$ with $\lambda \in (0, 1], \mu, \bar{\mu} \in \mathbb{C} \setminus \mathbb{R}$.
- Case III $\text{diag}(1, \lambda, \mu, \mu)$ with $\lambda \in (0, 1], \mu \in [-1, 1), \mu \neq 0, \mu \neq \lambda$.
- Case IV $\text{diag}(1, \lambda, \lambda, \lambda)$ with $\lambda \in (0, 1]$.

Proof: Since M is diagonalizable and 1 is an eigenvalue, we can write $\text{diag}(1, \lambda_1, \lambda_2, \lambda_3)$ for the diagonal form. If M has a negative eigenvalue, it must have multiplicity 2 by Proposition 2.5. Thus, M has at most one negative eigenvalue. On the other hand, since M is a real matrix, non-real eigenvalues of M come in conjugate pairs. These considerations give rise to Case II and Case III. Any other possibility corresponds to a Markov matrix, with all the eigenvalues real and positive. Finally, we claim that if the diagonal form is $\text{diag}(1, \lambda, \mu, \mu)$ with $\lambda \neq \mu$, then $\mu \neq 1$. Indeed, if $\mu = 1$, then $M - \text{Id}$ would have rank 1 because M is diagonalizable. Note that the rows of $M - \text{Id}$ vanish, which contradicts the fact that $M - \text{Id}$ has no negative entries outside the diagonal. We are led to either $\mu = \lambda$ (Case IV) or that the three eigenvalues are pairwise distinct (Case I). □

Next, we proceed to study the embeddability of Markov matrices lying in each of the cases in Lemma 5.1.

Case I.

Lemma 5.2. *Let M be as in Case I with an eigendecomposition $P \text{diag}(1, \lambda_1, \lambda_2, \lambda_3) P^{-1}$ with $\lambda_1, \lambda_2, \lambda_3 \in (0, 1]$ pairwise distinct and $P \in GL_4(\mathbb{R})$. Then M is embeddable if and only if $\text{Log}(M)$ is a rate matrix. Moreover, in this case $\text{Log}(M)$ is the only Markov generator.*

Proof: If $\lambda_1, \lambda_2, \lambda_3 \neq 1$, the embeddability of this case is already solved by Corollary 2.8. Otherwise, we can assume $\lambda_1 = 1$ without loss of

generality. Under this assumption, let Q be a Markov generator for M . By Remark 2.4(i), the eigenvalues of Q are $\log_{k_1}(1)$, $\log_{k_2}(1)$, $\log_{k_3}(\lambda_2)$, $\log_{k_4}(\lambda_3)$ for some $k_i \in \mathbb{Z}$. Since the sum of the rows of Q vanish, 0 is an eigenvalue of Q and therefore either $k_1 = 0$ or $k_2 = 0$. Using that Q is real we deduce that both of them are 0 because non-real eigenvalues of Q must appear in conjugate pairs. Again, since Q is real, the eigenvalues of Q corresponding to the non-repeated real eigenvalues of M are their respective principal logarithms, so that $k_3 = k_4 = 0$. As $\text{Log}(M)$ is the only logarithm whose eigenvalues are the principal logarithms of the eigenvalues of M we get $Q = \text{Log}(M)$. \square

Case II. Markov matrices M in Case II have non-real eigenvalues and an eigendecomposition as

$$(6) \quad M = P \text{diag}(1, \lambda, \mu, \bar{\mu})P^{-1} \text{ with } \lambda \in (0, 1], \mu \in \mathbb{C} \setminus \mathbb{R}, \text{ and } P \in GL_4(\mathbb{C}).$$

Without loss of generality, we assume $\text{Im}(\mu) > 0$ in order to simplify the notation used in this section. If $\lambda \neq 1$, Proposition 4.3 claims that the Markov generators of these matrices are of the form

$$\begin{aligned} \text{Log}_k(M) &= P \text{diag}(0, \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)})P^{-1} \\ &= P \text{diag}(0, \log(\lambda), \log(\mu) + 2\pi k i, \overline{\log(\mu)} - 2\pi k i)P^{-1}. \end{aligned}$$

The next result shows that the Markov generators are of this form even if $\lambda = 1$.

Proposition 5.3. *Let M be a Markov matrix with an eigendecomposition $P \text{diag}(1, 1, \mu, \bar{\mu})P^{-1}$ with $\mu, \bar{\mu} \in \mathbb{C}$ such that $\mu \neq 0$ and $\text{Im}(\mu) > 0$. Then,*

- (i) *If $\tilde{P} \text{diag}(1, 1, \mu, \bar{\mu})\tilde{P}^{-1}$ is another eigendecomposition of M ,*
 $P \text{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})P^{-1} = \tilde{P} \text{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})\tilde{P}^{-1}.$
- (ii) *A matrix Q is a real logarithm of M with rows summing to 0 if and only if Q has the form*

$$\text{Log}_k(M) = P \text{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})P^{-1}.$$

Proof: (i) If $\tilde{P} \text{diag}(1, 1, \mu, \bar{\mu})\tilde{P}^{-1}$ is another eigendecomposition of M , then $\tilde{P} = PA$ for some matrix $A \in \text{Comm}^*(\text{diag}(1, 1, \mu, \bar{\mu}))$. As

$$\text{Comm}^*(\text{diag}(1, 1, \mu, \bar{\mu})) = \text{Comm}^*(\text{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})),$$

we obtain the desired result.

(ii) By (i), the definition of $\text{Log}_k(M)$ does not depend on P and it is a logarithm of M (see Theorem 2.3). Note that $(1, 1, 1, 1)^t$ is an eigenvector

of M with eigenvalue 1 because M is a Markov matrix. Hence we can assume that the first column vector of P is $(1, 1, 1, 1)^t$ and the rows of $\text{Log}_k(M)$ sum to 0.

Conversely, we prove now that any real logarithm Q of M with rows summing to 0 is of the form $\text{Log}_k(M)$. From Theorem 2.3 we have that

$$Q = P A \text{diag}(\log_{k_1}(1), \log_{k_2}(1), \log_{k_3}(\mu), \log_{k_4}(\bar{\mu})) A^{-1} P^{-1}$$

for some $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ and some $A \in \text{Comm}^*(\text{diag}(1, 1, \mu, \bar{\mu}))$. Since the rows of Q sum to 0 we get $k_1 = k_2 = 0$ as in the proof of Lemma 5.2. As Q is real, we get that $\log_{k_3}(\mu)$ and $\log_{k_4}(\bar{\mu})$ must be conjugate pairs: $\log_{k_4}(\bar{\mu}) = \overline{\log_{k_3}(\mu)} = \log_{-k_3}(\bar{\mu})$ and hence, $k_4 = -k_3$. Since the matrix A commutes with $(0, 0, \log_{k_3}(\mu), \overline{\log_{k_3}(\mu)})$ (see Remark 2.2), Q is equal to $\text{Log}_k(M)$ (taking $k = k_3$). \square

Now that we know that all logarithms in Case II are of type $\text{Log}_k(M)$, in order to proceed with the study of embeddability we decompose $\text{Log}_k(M)$ as

$$(7) \quad \text{Log}_k(M) = \text{Log}(M) + k \cdot V, \text{ where } V = P \text{diag}(0, 0, 2\pi i, -2\pi i) P^{-1}.$$

Next we show that the values of k for which $\text{Log}_k(M)$ is a Markov generator form a sequence of consecutive numbers.

Lemma 5.4. *Let M be a Markov matrix as in (6). If $\text{Log}_{k_1}(M)$ and $\text{Log}_{k_2}(M)$ are rate matrices with $k_1 < k_2$, then $\text{Log}_k(M)$ is a rate matrix for all $k \in [k_1, k_2]$.*

Proof: The proof is immediate because the entries of $\text{Log}_k(M) = \text{Log}(M) + k \cdot V$ depend linearly on k . \square

Note that we could use Lemma 3.1 to bound the values of k for which $\text{Log}_k(M)$ might be a Markov generator, as we did in Section 4. However, Lemma 5.4 allows a precise description of those logarithms of M that are Markov generators (not only giving a necessary condition).

Theorem 5.5. *Let M , P , and V be as above. Define*

$$\mathcal{L} := \max_{(i,j): i \neq j, V_{i,j} > 0} \left[-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \right], \quad \mathcal{U} := \min_{(i,j): i \neq j, V_{i,j} < 0} \left[-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \right]$$

and set $\mathcal{N} := \{(i, j) : i \neq j, V_{i,j} = 0, \text{ and } \text{Log}(M)_{i,j} < 0\}$.

Then, $\text{Log}_k(M)$ is a rate matrix if and only if $\mathcal{N} = \emptyset$ and $\mathcal{L} \leq k \leq \mathcal{U}$.

Proof: By (7) we have that $\text{Log}_k(M) = \text{Log}(M) + k \cdot V$. Now, assume we choose $k \in \mathbb{Z}$ such that $\text{Log}_k(M)$ is a rate matrix. In this case, $\text{Log}(M)_{i,j} + kV_{i,j} \geq 0$ for all $i \neq j$. Hence, for $i \neq j$ we have:

- $0 \leq \text{Log}(M)_{i,j}$ for all i, j such that $V_{i,j} = 0$. In particular, $\mathcal{N} = \emptyset$.
- $-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \leq k$ for all i, j such that $V_{i,j} > 0$. In particular, $\mathcal{L} \leq k$.
- $-\frac{\text{Log}(M)_{i,j}}{V_{i,j}} \geq k$ for all i, j such that $V_{i,j} < 0$. In particular, $\mathcal{U} \geq k$.

Conversely, let us assume that $\mathcal{N} = \emptyset$ and that there is $k \in \mathbb{Z}$ such that $\mathcal{L} \leq k \leq \mathcal{U}$. We want to check that $\text{Log}_k(M)$ is a rate matrix. Indeed, take (i, j) with $i \neq j$, then:

- If $V_{i,j} = 0$, we have $\text{Log}_k(M)_{i,j} = \text{Log}(M)_{i,j}$. Since $\mathcal{N} = \emptyset$ it follows that $\text{Log}(M)_{i,j} \geq 0$, thus $\text{Log}_k(M)_{i,j} \geq 0$.
- If $V_{i,j} > 0$, then $\text{Log}_k(M)_{i,j} \geq \text{Log}(M)_{i,j} + \mathcal{L} \cdot V_{i,j} \geq \text{Log}(M)_{i,j} + \frac{-\text{Log}(M)_{i,j}}{V_{i,j}} V_{i,j} = 0$.
- If $V_{i,j} < 0$, then $-\text{Log}_k(M)_{i,j} \leq -\text{Log}(M)_{i,j} - \mathcal{U} \cdot V_{i,j} \leq -\text{Log}(M)_{i,j} - \frac{-\text{Log}(M)_{i,j}}{V_{i,j}} V_{i,j} = 0$. Moreover, the rows of $\text{Log}_k(M)$ sum to 0, as proved in Propositions 4.3 and 5.3. \square

The theorem above lists all Markov generators of M . As an immediate consequence, we get the following characterization of 4×4 embeddable matrices with a conjugate pair of (non-real) eigenvalues.

Corollary 5.6. *Let $M = P \text{diag}(1, \lambda, \mu, \bar{\mu}) P^{-1}$ for some $\lambda \in (0, 1]$ and $\mu, \bar{\mu} \in \mathbb{C} \setminus \mathbb{R}$. Let \mathcal{L}, \mathcal{U} , and \mathcal{N} be as in Theorem 5.5. Then, M is embeddable if and only if $\mathcal{N} = \emptyset$ and $\mathcal{L} \leq \mathcal{U}$.*

Now we can prove Theorem 1.1 in the introduction using Lemma 5.2 and Corollary 5.6:

Proof of Theorem 1.1: Assume that $M = P \text{diag}(1, \lambda_1, \lambda_2, \lambda_3) P^{-1}$ is a 4×4 Markov matrix with $\lambda_1 \in \mathbb{R}_{>0}$, $\lambda_2 \in \mathbb{C}$, $\lambda_3 \in \mathbb{C}$ pairwise distinct. We know that $|\lambda_i| \leq 1$ and, if M is embeddable, $\lambda_i \notin \mathbb{R}_{\leq 0}$ for any $i = 1, 2, 3$. Therefore, M lies in Case I if all its eigenvalues are real and in Case II otherwise.

If M lies in Case I, then M is embeddable if and only if $\text{Log}(M)$ is a rate matrix (Lemma 5.2). As the rows of the principal logarithm of a Markov matrix sum to 0, by setting $V = 0$ we have that $\text{Log}(M)$ is a rate matrix if and only if $\mathcal{N} = \emptyset$. Moreover, in this case $\text{Log}(M)$ is the only Markov generator (Lemma 5.2).

If M lies in Case II, then the statement is precisely Corollary 5.6. In addition, from Theorem 5.5 we obtain that the Markov generators in this case are $\text{Log}_k(M)$ for $k \in [\mathcal{L}, \mathcal{U}]$, which coincide with $\text{Log}(M) + 2\pi k V$ as defined in the statement of Theorem 1.1. \square

Next, we present an algorithm that solves both the embedding problem and the rate identifiability problem for 4×4 Markov matrices in Cases I and II.

Remark 5.7. We already know that the embeddability of a Markov matrix is not always determined by the principal logarithm [5]. In the 4×4 case, we can prove that the set of embeddable Markov matrices whose principal logarithm is not a Markov generator is not a subset of zero measure; on the contrary, it is a set of full dimension. Moreover, for any $k \in \mathbb{Z}$ there is a non-empty Euclidean open set of *embeddable* Markov matrices, all of them in Case II, whose unique Markov generator is $\text{Log}_k(M)$. See [6] for details.

Algorithm 5.8.

```

input :  $M$ , a  $4 \times 4$  Markov matrix with distinct eigenvalues as in
          Theorem 1.1.
output: All its Markov generators if  $M$  is embeddable, an empty
          list otherwise.

generators = [ ]
compute eigenvalues of  $M$ 
if  $M$  has no negative or zero eigenvalue, then
  set  $\text{Principal} = \text{Log}(M)$ 
  if all the eigenvalues are real, then
     $\lfloor$  add  $\text{Principal}$  to generators if it is a rate matrix
  else
    compute  $P$  and  $V$  as in Theorem 1.1
    compute  $\mathcal{L}$ ,  $\mathcal{U}$ , and  $\mathcal{N}$ 
    if  $\mathcal{N} = \emptyset$ , then
      for  $k \in \mathbb{Z}$  such that  $\mathcal{L} \leq k \leq \mathcal{U}$  do
         $\lfloor$  compute  $\text{Log}_k(M) = \text{Principal} + kV$ 
         $\lfloor$  add  $\text{Log}_k(M)$  to generators if it is a rate matrix
    if  $\text{generators} = [ ]$ , then
       $\lfloor$  return " $M$  not embeddable"
    else
       $\lfloor$  return generators

```

Case III. Let M be a Markov matrix as in Case III with an eigendecomposition as

$$(8) \quad M = P \text{diag}(1, \lambda, \mu, \mu) P^{-1} \text{ with } \lambda \in (0, 1], \mu \in [-1, 1), \mu \neq \lambda, 0, \\ \text{and } P \in GL_4(\mathbb{R}).$$

Note that the matrix P can be assumed to be real since all the eigenvalues of M are real. Note also that this case can be seen as a limit case of

Markov matrices with a conjugate pair of complex eigenvalues (Case II) and, analogously to that case, M has infinitely many real logarithms with rows summing to 0. However, in the present case one has to be careful when using Theorem 2.3 in order to take into account the commutant of the diagonal form of M .

We introduce the following matrices.

Definition 5.9. Let M, P, λ , and μ be as in (8) above. For any $k \in \mathbb{Z}$ and $x, y, z \in \mathbb{R}$, we define the matrix

$$Q_k(x, y, z) = L + (2\pi k + \text{Arg}(\mu))V(x, y, z),$$

where $L = P \text{diag}(0, \log(\lambda), \log |\mu|, \log |\mu|)P^{-1}$ and

$$V(x, y, z) := P \text{diag} \left(0, 0, \begin{pmatrix} -y & x \\ -z & y \end{pmatrix} \right) P^{-1}.$$

Remark 5.10. If $\mu > 0$, we have $Q_0(x, y, z) = \text{Log}(M)$ for all $(x, y, z) \in \mathbb{R}^3$. For later use, note that $V(ax, ay, az) = aV(x, y, z)$ for all $a \in \mathbb{R}$, and hence

$$Q_k(x, y, z) = \begin{cases} Q_{-k}(-x, -y, -z) & \text{if } \mu > 0, \\ Q_{-k-1}(-x, -y, -z) & \text{if } \mu < 0. \end{cases}$$

As in the previous case, we start by enumerating all the real logarithms of M with rows summing to 0. To this end, we define $\mathcal{V} \subset \mathbb{R}^3$ as the algebraic variety

$$\mathcal{V} = \{(x, y, z) \in \mathbb{R}^3 \mid xz - y^2 = 1\}.$$

The next theorem shows that those logarithms with real entries and rows summing to 0 are of the form $Q_k(x, y, z)$ with $(x, y, z) \in \mathcal{V}$. Furthermore, \mathcal{V} is a 2-sheet hyperboloid with one of its sheets \mathcal{V}_- in the orthant $x, z < 0$ and the other sheet \mathcal{V}_+ in the orthant $x, z > 0$. The restriction of (x, y, z) to either of these components gives a bijection between the set of matrices $Q_k(x, y, z)$ and the real logarithms of Q with rows summing to 0 (other than $\text{Log}(M)$).

Theorem 5.11. *Let M be a Markov matrix as in (8). Then, the following are equivalent:*

- (i) Q is a real logarithm of M with rows summing to 0,
- (ii) $Q = Q_k(x, y, z)$ for some $(x, y, z) \in \mathcal{V}$, $k \in \mathbb{Z}$.

Moreover, if $Q \neq \text{Log}(M)$, there is a unique $k \in \mathbb{Z}$ and a unique $(x, y, z) \in \mathcal{V}_+$ such that $Q = Q_k(x, y, z)$.

Proof: (i) \Rightarrow (ii) We know by Theorem 2.3 that any logarithm Q of M is of type

$$Q = P A \operatorname{diag}(\log_{k_1}(1), \log_{k_2}(\lambda), \log_{k_3}(\mu), \log_{k_4}(\mu)) A^{-1} P^{-1}$$

for some $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ and some $A \in \operatorname{Comm}^*(\operatorname{diag}(1, \lambda, \mu, \mu))$.

Since the rows of Q sum to 0, $(1, 1, 1, 1)^t$ is an eigenvector of M with eigenvalue 0. Since non-real eigenvalues of Q must appear in conjugate pairs it follows that $k_1 = k_2 = 0$ (even if $\lambda = 1$). Moreover, we also deduce that $\log_{k_3}(\mu)$ and $\log_{k_4}(\mu)$ are a conjugate pair. This implies that $k_4 = -k_3$ if $\mu > 0$ and $k_4 = -k_3 - 1$ if $\mu < 0$. Therefore, if we take $k = k_3$, we have

$$\begin{aligned} Q &= P A \operatorname{diag}(\log(1), \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)}) A^{-1} P^{-1} \\ (9) \quad &= P A \operatorname{diag}(0, \log(\lambda), \log|\mu| + (2\pi k + \operatorname{Arg}(\mu))i, \log|\mu| \\ &\quad - (2\pi k + \operatorname{Arg}(\mu))i) A^{-1} P^{-1}. \end{aligned}$$

If all the eigenvalues of Q are real, we deduce that $\operatorname{Arg}(\mu) = 0$ and $k = 0$. In this case, the eigenvalues of Q are given by the principal logarithm of the respective eigenvalues of M and hence $Q = \operatorname{Log}(M)$.

Now assume that Q has a conjugate pair of complex eigenvalues $\log|\mu| \pm (2\pi k + \operatorname{Arg}(\mu))i$. Hence, the third and fourth column vectors of PA must be a conjugate pair (up to scalar). Furthermore, we have that P is a real matrix and hence it is the third and fourth column vectors of A that are a conjugate pair. This fact together with the fact that A commutes with $\operatorname{diag}(1, \lambda, \mu, \mu)$ leads to:

$$A = \begin{pmatrix} z_1 & 0 & 0 & 0 \\ 0 & z_2 & 0 & 0 \\ 0 & 0 & a + bi & z(a - bi) \\ 0 & 0 & c + di & z(c - di) \end{pmatrix}$$

with $z, z_1, z_2 \in \mathbb{C} \setminus \{0\}$ and $a, b, c, d \in \mathbb{R}$ satisfying $ad - bc \neq 0$ because A is a non-singular matrix. We can decompose A as $A = A_1 A_2$, where:

$$(10) \quad A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix}, \quad A_2 = \begin{pmatrix} z_1 & 0 & 0 & 0 \\ 0 & z_2 & 0 & 0 \\ 0 & 0 & 1 & z \\ 0 & 0 & i & -zi \end{pmatrix}.$$

Let us define

$$(11) \quad J := A_2 \operatorname{diag}(0, \log(\lambda), \log |\mu| + (2\pi k + \operatorname{Arg}(\mu))i, \log |\mu| - (2\pi k + \operatorname{Arg}(\mu))i) A_2^{-1}$$

$$(12) \quad = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \log(\lambda) & 0 & 0 \\ 0 & 0 & \log |\mu| & 2\pi k + \operatorname{Arg}(\mu) \\ 0 & 0 & -(2\pi k + \operatorname{Arg}(\mu)) & \log |\mu| \end{pmatrix}.$$

Using this notation, the matrix Q in (9) can be written as $Q = PA_1JA_1^{-1}P^{-1}$. Note that A_1 commutes with $\operatorname{diag}(0, \log(\lambda), \log |\mu|, \log |\mu|)$ and hence

$$Q = P \operatorname{diag}(0, \log(\lambda), \log |\mu|, \log |\mu|) P^{-1} + (2\pi k + \operatorname{Arg}(\mu)) P A_1 \operatorname{diag} \left(0, 0, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right) A_1^{-1} P^{-1}.$$

A final computation shows that $A_1 \operatorname{diag}(0, 0, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}) A_1^{-1}$ equals $V(x, y, z)$ with

$$x = \frac{a^2 + b^2}{ad - bc}, \quad y = \frac{ac + bd}{ad - bc}, \quad z = \frac{c^2 + d^2}{ad - bc}.$$

It is immediate to show that $xz - y^2 = 1$, thus $(x, y, z) \in \mathcal{V}$. This proves that (i) implies (ii).

(ii) \Rightarrow (i) We know that $Q_k(x, y, z)$ is real by Definition 5.9: it is straightforward to check that $(1, 1, 1, 1)^t$ is an eigenvector with eigenvalue 0 of both L and V , and so it is also an eigenvector of $Q_k(x, y, z)$ with eigenvalue 0.

Hence it is enough to check that if $(x, y, z) \in \mathcal{V}$, then $Q_k(x, y, z)$ is a logarithm of M . To this end, consider the matrix J introduced in (12) and the matrix

$$B := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{y}{x} & \frac{1}{x} \end{pmatrix}.$$

If $(x, y, z) \in \mathcal{V}$, then we have $z = \frac{1+y^2}{x}$. A straightforward computation shows that $P^{-1}Q_k(x, y, \frac{1+y^2}{x})P - BJB^{-1} = 0$. Hence, it follows from (11) that

$$Q_k \left(x, y, \frac{1+y^2}{x} \right) = PA \operatorname{diag}(0, \log(\lambda), \log|\mu| + (2\pi k + \operatorname{Arg}(\mu))i, \log|\mu| - (2\pi k + \operatorname{Arg}(\mu))i)A^{-1}P^{-1}$$

with $A = BA_2$ (A_2 is defined in (10)). Since both B and A_2 commute with $\operatorname{diag}(1, \lambda, \mu, \mu)$ it follows from Theorem 2.3 that $Q_k(x, y, \frac{1+y^2}{x})$ is a logarithm of M , which concludes the first part of the proof.

In the first part of the proof, we already proved that there exists $k \in \mathbb{Z}$ and $(x, y, z) \in \mathcal{V}$ such that $Q = Q_k(x, y, z)$. By Remark 5.10, we can take $(x, y, z) \in \mathcal{V}_+$ without loss of generality. To prove that k and (x, y, z) are unique we assume that $Q_k(x, y, z) = Q_{\tilde{k}}(\tilde{x}, \tilde{y}, \tilde{z})$ for some $\tilde{k} \in \mathbb{Z}$ and $(\tilde{x}, \tilde{y}, \tilde{z}) \in \mathcal{V}_+$. In this case, we have

$$(2\pi k + \operatorname{Arg}(\mu))V(x, y, z) = (2\pi\tilde{k} + \operatorname{Arg}(\mu))V(\tilde{x}, \tilde{y}, \tilde{z}).$$

Since $Q \neq \operatorname{Log}(M)$ then $(2\pi k + \operatorname{Arg}(\mu)) \neq 0$ and hence:

$$x = \frac{2\pi\tilde{k} + \operatorname{Arg}(\mu)}{2\pi k + \operatorname{Arg}(\mu)}\tilde{x}, \quad y = \frac{2\pi\tilde{k} + \operatorname{Arg}(\mu)}{2\pi k + \operatorname{Arg}(\mu)}\tilde{y}, \quad z = \frac{2\pi\tilde{k} + \operatorname{Arg}(\mu)}{2\pi k + \operatorname{Arg}(\mu)}\tilde{z}.$$

Now, using that $(x, y, z), (\tilde{x}, \tilde{y}, \tilde{z}) \in \mathcal{V}$ we get $xz - y^2 = \left(\frac{2\pi\tilde{k} + \operatorname{Arg}(\mu)}{2\pi k + \operatorname{Arg}(\mu)}\right)^2(\tilde{x}\tilde{z} - \tilde{y}^2) = 1$. Moreover, since $x, z, \tilde{x}, \tilde{z} > 0$, we deduce that $\frac{2\pi\tilde{k} + \operatorname{Arg}(\mu)}{2\pi k + \operatorname{Arg}(\mu)} = 1$, so $\tilde{k} = k$ and $(\tilde{x}, \tilde{y}, \tilde{z}) = (x, y, z)$. □

Remark 5.12. Because of Remark 5.10, every real logarithm of M with rows summing to 0 can also be realized as some $Q_k(x, y, z)$ for a unique $k \in \mathbb{Z}$ and a unique $(x, y, z) \in \mathcal{V}_-$.

In order to characterize those logarithms that are rate matrices, for any $k \in \mathbb{Z}$ we define the set

$$\mathcal{P}_k = \{(x, y, z) \in \mathbb{R}^3 : Q_k(x, y, z) \text{ is a rate matrix}\}.$$

Note that the entries of $Q_k(x, y, z)$ depend linearly on x, y, z , and hence \mathcal{P}_k is the space of solutions to a system of linear inequalities (i.e. a convex polyhedron). From Theorem 5.11 we obtain that the set of Markov generators for a Markov matrix in Case III is $\bigcup_k \mathcal{P}_k \cap \mathcal{V}_+$. The following corollary is an immediate consequence of Lemma 3.1 and Theorem 5.11 and shows that there is a finite set of integers k such that $\mathcal{P}_k \cap \mathcal{V}_+ \neq \emptyset$.

In Appendix A we show a procedure to check whether the intersection $\mathcal{P}_k \cap \mathcal{V}_+$ is not empty and get a point in it.

Using the notation introduced in Section 4, if Q is a Markov generator of a Markov matrix M with eigenvalues $1, \lambda,$ and μ as in (8), then it has at most one conjugate pair of non-real eigenvalues, $\log_k(\mu)$ and $\overline{\log_k(\mu)}$. It follows from Lemma 3.1 that their imaginary part is bounded by $\beta_4(\mu) = -\log|\mu|$ and as a consequence, we obtain the next result.

Corollary 5.13. *Let M be a Markov matrix as in (8). If Q is a Markov generator of M , then $Q = Q_k(x, y, z)$ for some $(x, y, z) \in \mathcal{V}_+$ and some $k \in \mathbb{Z}$ satisfying*

$$\frac{-\operatorname{Arg}(\mu) + \log|\mu|}{2\pi} \leq k \leq \frac{-\operatorname{Arg}(\mu) - \log|\mu|}{2\pi}.$$

As a byproduct, we give an embeddability criterion for 4×4 Markov matrices with two repeated eigenvalues.

Corollary 5.14. *Let M be a Markov matrix as in (8).*

- (i) *If $\mu > 0$, M is embeddable if and only if $\mathcal{P}_k \cap \mathcal{V}_+ \neq \emptyset$ for some k with*

$$\left\lceil \frac{\log|\mu|}{2\pi} \right\rceil \leq k \leq \left\lfloor \frac{-\log|\mu|}{2\pi} \right\rfloor.$$

- (ii) *If $\mu < 0$, M is embeddable if and only if $\mathcal{P}_k \cap \mathcal{V}_+ \neq \emptyset$ for some k satisfying*

$$\left\lceil -\frac{1}{2} + \frac{\log|\mu|}{2\pi} \right\rceil \leq k \leq \left\lfloor -\frac{1}{2} - \frac{\log|\mu|}{2\pi} \right\rfloor.$$

In particular, if $\mu < -e^{-\pi}$, then M is not embeddable.

Proof: Since $k \in \mathbb{Z}$, the bounds on k are a straightforward consequence of Corollary 5.13. Indeed, it is enough to take $\operatorname{Arg}(\mu) = 0$ for $\mu > 0$ and $\operatorname{Arg}(\mu) = \pi$ for $\mu < 0$. In the case of $\mu < 0$, it is immediate to check that $\left\lceil -\frac{1}{2} + \frac{\log|\mu|}{2\pi} \right\rceil \leq \left\lfloor -\frac{1}{2} - \frac{\log|\mu|}{2\pi} \right\rfloor$ if and only if $\log|\mu| < -\pi$. Hence, if $\mu < -e^{-\pi}$, there is no k satisfying the embeddability conditions in the statement. □

Remark 5.15. Example 4.3 in [5] shows an embeddable Markov matrix as in (8) with $\mu = -e^{-\pi}$. Thus, the bound on Corollary 5.14 is sharp.

From Corollary 5.14 we derive an algorithm that tests the embeddability of Markov matrices lying in Case III.

Algorithm 5.16 (Markov generators of 4×4 matrices with two repeated eigenvalues).

```

input :  $M$  (Markov matrix) and  $P$  as in (8).
output: One of its Markov generators  $Q_k(x, y, z)$  for each  $k \in \mathbb{Z}$ 
         (if they exist).

generators = [ ]
compute the eigenvalues of  $M$ :  $1, \lambda, \mu, \mu$ 
if  $\det(M) > 0$  and  $\mu \geq -e^{-\pi}$ , then
    Compute  $L = P \operatorname{diag}(0, \log(\lambda), \log|\mu|, \log|\mu|)P^{-1}$ 
    set  $\mathcal{L} = \lceil \frac{-\operatorname{Arg}(\mu) + \log|\mu|}{2\pi} \rceil$  and  $\mathcal{U} = \lfloor \frac{-\operatorname{Arg}(\mu) - \log|\mu|}{2\pi} \rfloor$ 
    for  $\mathcal{L} \leq k \leq \mathcal{U}$  ( $k \in \mathbb{Z}$ ): do
        if  $\mathcal{P}_k \cap \mathcal{V} \neq \emptyset$  (see Appendix A), then
            choose  $(x, y, z) \in \mathcal{P}_k \cap \mathcal{V}_+$  (see Appendix A)
            add  $Q_k(x, y, z) = L + kV(x, y, z)$  to generators
    if generators = [ ], then
        return “ $M$  not embeddable”
    else return generators
    
```

Remark 5.17. If $Q_k(x, y, z) \neq \operatorname{Log}(M)$, then each choice of $(x, y, z) \in \mathcal{P}_k \cap \mathcal{V}_+$ in the algorithm above would give a different Markov generator for M (5.11). Thus, the set of all Markov generators of M is obtained by considering, for each possible k , all $(x, y, z) \in \mathcal{P}_k \cap \mathcal{V}_+$ (this can produce infinitely many Markov generators). In Appendix A we show how to compute $\#\mathcal{P}_k \cap \mathcal{V}_+$ for a fixed k .

Case IV. Here, we deal with 4×4 Markov matrices with an eigenvalue of multiplicity 3 or 4. This case corresponds to the *equal-input* matrices used in phylogenetics. The reader is referred to [1] and [2] for a recent and parallel study on this class of matrices with special emphasis on embeddability.

Proposition 5.18. *Let M be a diagonalizable 4×4 Markov matrix with eigenvalues $1, \lambda, \lambda, \lambda$. Then the following are equivalent:*

- (i) M is embeddable.
- (ii) $\det(M) > 0$.
- (iii) $\operatorname{Log}(M)$ is a rate matrix.

Proof: If $M = \operatorname{Id}$, that is, $\lambda = 1$, then it follows from Theorem 2.3 that $\operatorname{Log}(M)$ is the zero matrix and hence it is a Markov generator for M . Moreover, it follows from Corollary 3.3 that the zero matrix is the only Markov generator of the identity matrix.

Now, let us assume $\lambda \neq 1$. Since $\det(e^Q) = e^{\text{tr}(Q)}$ it follows that (i) \Rightarrow (ii). (iii) \Rightarrow (i) is straightforward, thus to conclude the proof it is enough to check that if $\det(M) > 0$, then $\text{Log}(M)$ is a rate matrix.

Since M is a Markov matrix we get that $M - \lambda \text{Id}$ is a rank 1 matrix whose rows sum to $1 - \lambda$. Hence:

$$(13) \quad M = \begin{pmatrix} a + \lambda & b & c & d \\ a & b + \lambda & c & d \\ a & b & c + \lambda & d \\ a & b & c & d + \lambda \end{pmatrix},$$

with $\lambda = 1 - (a + b + c + d) \in (0, 1)$, $a, b, c, d \geq 0$.

Let us fix $S \in GL_4(\mathbb{R})$ such that $M = S \text{diag}(1, \lambda, \lambda, \lambda) S^{-1}$. Note that if $\lambda = 1$, then $M = \text{Id}$ and $\text{Log}(M) = 0$ is a rate matrix. On the other hand, if $\lambda \in (0, 1)$, then we have:

$$\begin{aligned} \text{Log}(M) &= S \text{diag}(0, \log(\lambda), \log(\lambda), \log(\lambda)) S^{-1} \\ &= \frac{\log(\lambda)}{\lambda - 1} (S \text{diag}(1, \lambda, \lambda, \lambda) S^{-1} - S \text{diag}(1, 1, 1, 1) S^{-1}) \\ &= \frac{\log(\lambda)}{\lambda - 1} (M - \text{Id}). \end{aligned}$$

Since $M - \text{Id}$ is a rate matrix and $\lambda \in (0, 1)$ it follows that $\text{Log}(M)$ is a rate matrix. \square

Remark 5.19. In the context of DNA nucleotide substitution models, these matrices correspond to the Felsenstein 81 model [12]. The stationary distribution of such matrices is given by $\Pi = (a, b, c, d)/(a + b + c + d)$, where a, b, c, d are as in (13) (in particular, $a + b + c + d > 0$). When the stationary distribution is uniform, that is, $a = b = c = d$, we recover the Jukes–Cantor model [23].

5.2. Embeddability of non-diagonalizable 4×4 Markov matrices. If we restrict the embedding problem to non-diagonalizable 4×4 matrices, we have:

Theorem 5.20. *A non-diagonalizable 4×4 Markov matrix is embeddable if and only if it has only positive eigenvalues and its principal logarithm is a rate matrix. In this case, it has just one Markov generator.*

Proof: The “if” part is immediate, so we proceed to prove the “only if” part. Let M be an embeddable non-diagonalizable 4×4 Markov matrix. We know that the dominant eigenvalue 1 has the same algebraic and

geometric multiplicity (see [25, §8.4]). Therefore, M has at most one Jordan block of size greater than 1 and, in this case, its Jordan form is one of the following:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \mu & 1 \\ 0 & 0 & 0 & \mu \end{pmatrix} \text{ with } \mu \neq 0, 1, \lambda \neq 0, \text{ or } \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda & 1 & 0 \\ 0 & 0 & \lambda & 1 \\ 0 & 0 & 0 & \lambda \end{pmatrix} \text{ with } \lambda \neq 0, 1.$$

As M is a real matrix, its eigenvalues are necessarily real. Moreover, as M is embeddable, Proposition 2.5 yields that λ and μ are positive. An immediate consequence of Theorem 2 in [8] is that if each Jordan block appears exactly once in its Jordan form, then the only possible real logarithm of M is the principal logarithm.

Hence, if M has a real logarithm other than $\text{Log}(M)$, then the Jordan form of M is $J := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \lambda & 1 \\ 0 & 0 & 0 & \lambda \end{pmatrix}$ with $\lambda \in (0, 1)$.

Take P such that $M = PJP^{-1}$. A more general version of Theorem 2.3 for non-diagonalizable matrices (see Theorem 1.27 in [19]) shows that any logarithm Q of M has the form:

$$Q = PA \begin{pmatrix} 2\pi k_1 i & 0 & 0 & 0 \\ 0 & 2\pi k_2 i & 0 & 0 \\ 0 & 0 & \log(\lambda) + 2\pi k_3 i & 1/\lambda \\ 0 & 0 & 0 & \log(\lambda) + 2\pi k_3 i \end{pmatrix} A^{-1} P^{-1}$$

for some $A \in \text{Comm}^*(J)$.

It follows that A can be written as $A = \text{diag}(B, \text{Id}_2) \text{diag}(c_1, c_2, c_3, c_3)$ with $B \in GL_2(\mathbb{C})$. Now, if Q is a rate matrix, it is a real matrix and hence $k_1 = -k_2$ and $k_3 = 0$. Moreover, its rows sum to 0 and hence 0 is an eigenvalue of Q . Hence, $k_1 = -k_2 = 0$. Thus:

$$\begin{aligned} Q &= PA \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \log(\lambda) & 1/\lambda \\ 0 & 0 & 0 & \log(\lambda) \end{pmatrix} A^{-1} P^{-1} \\ &= P \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \log(\lambda) & 1/\lambda \\ 0 & 0 & 0 & \log(\lambda) \end{pmatrix} P^{-1}, \end{aligned}$$

and we see that the eigenvalues of Q are the principal logarithms of the eigenvalues of M , so that $Q = \text{Log}(M)$. □

6. Rate identifiability

Once we know that a Markov matrix arises from a continuous-time model, we want to determine its corresponding substitution rates. In other words, given an embeddable matrix we want to know if we can uniquely identify its Markov generator. Corollary 3.3 shows that if the determinant of the Markov matrix is big enough, then there is just one generator. However, this is not the case if the determinant is small. Note that a small determinant means that the substitution rates are large or that the substitution process ruled by M has taken a lot of time.

Definition 6.1. An embeddable Markov matrix M has *identifiable rates* if there exists a unique rate matrix Q such that $M = e^Q$. The *rate identifiability problem* consists in deciding whether a given Markov matrix has identifiable rates or not.

Proposition 6.2. *Let M be a diagonalizable 4×4 embeddable Markov matrix with eigenvalues $1, \lambda, \lambda, \lambda$. If $\det(M) > e^{-6\pi}$, the rates of M are identifiable and the only generator is $\text{Log}(M)$.*

Proof: Let Q be a Markov generator for M . If $\lambda > e^{-2\pi}$, then the real part of the non-zero eigenvalues of Q is greater than -2π , thus it follows from Lemma 3.1 that their imaginary part lies in the interval $(-2\pi, 2\pi)$. Since the eigenvalues of M are real and positive this implies that the non-zero eigenvalues of Q are $\log(\lambda)$ and hence $Q = \text{Log}(M)$. □

Remark 6.3. We do not think that this bound is sharp. To our knowledge, the largest determinant of a 4×4 embeddable matrix with three repeated eigenvalues and non-identifiable rates is $e^{-12\pi}$, and corresponds to the matrix:

$$M = \frac{1}{4} \begin{pmatrix} 1 + 3e^{-4\pi} & 1 - e^{-4\pi} & 1 - e^{-4\pi} & 1 - e^{-4\pi} \\ 1 - e^{-4\pi} & 1 + 3e^{-4\pi} & 1 - e^{-4\pi} & 1 - e^{-4\pi} \\ 1 - e^{-4\pi} & 1 - e^{-4\pi} & 1 + 3e^{-4\pi} & 1 - e^{-4\pi} \\ 1 - e^{-4\pi} & 1 - e^{-4\pi} & 1 - e^{-4\pi} & 1 + 3e^{-4\pi} \end{pmatrix}.$$

Next we show three Markov generators for it:

$$\begin{pmatrix} -3\pi & \pi & 2\pi & 0 \\ \pi & -3\pi & 0 & 2\pi \\ 0 & 2\pi & -3\pi & \pi \\ 2\pi & 0 & \pi & -3\pi \end{pmatrix}, \quad \begin{pmatrix} -3\pi & \pi & \pi & \pi \\ \pi & -3\pi & \pi & \pi \\ \pi & \pi & -3\pi & \pi \\ \pi & \pi & \pi & -3\pi \end{pmatrix},$$

$$\begin{pmatrix} -3\pi & \pi & 0 & 2\pi \\ \pi & -3\pi & 2\pi & 0 \\ 2\pi & 0 & -3\pi & \pi \\ 0 & 2\pi & \pi & -3\pi \end{pmatrix}.$$

Note that Theorem 4.5 bounds the number of generators of a Markov matrix with no repeated eigenvalues. Moreover, Algorithm 4.7 lists all the generators of such a matrix. If we restrict the identifiability problem to 4×4 Markov matrices, we are able to deal with the rate identifiability problem for all the matrices in Cases I, II, and III, that is, all 4×4 matrices except those with an eigenvalue of multiplicity 3 (Case IV), for which we have Proposition 6.2. This is summarized in the following table:

Diagonal form of M	Embeddability criterion	Number of generators
Case I	$\text{Log}(M)$ is a rate matrix	1
Case II	$\mathcal{N} = \emptyset$ and $\mathcal{L} \leq \mathcal{U}$ (Corollary 5.6)	$\mathcal{U} - \mathcal{L} + 1$ (Theorem 5.5)
Case III	$\bigcup_k (\mathcal{P}_k \cap \mathcal{V}) \neq \emptyset$ (Corollary 5.14)	$\sum_k \#(\mathcal{P}_k \cap \mathcal{V})$ (Remark 5.17)
Case IV	$\det(M) > 0$ (Proposition 5.18)	1 if $\det(M) > e^{-6\pi}$
M does not diagonalize	$\text{Log}(M)$ is a rate matrix (Theorem 5.20)	1 (Theorem 5.20)
Other diagonal forms	M is not embeddable	—

TABLE 2. Embeddability test and number of generators for a 4×4 Markov matrix depending on its diagonal form.

7. Discussion

In this paper we have studied the embeddability and rate identifiability of Markov matrices. Our study has led to a number of results and the development of algorithms that are able to test the embeddability and list the Markov generators of a given Markov matrix, namely Algorithm 4.7 for any size n , and Algorithm 5.8 specifically for $n = 4$. In this case, the embedding problem has been completely solved. It seems natural to think that the next step is to extend the study to 5×5 matrices, at the expense of having to consider two conjugate pairs of complex eigenvalues instead of one and dealing with the difficulties that this causes. Most of our results of Section 5 have an immediate generalization to Markov matrices with a single conjugate pair of eigenvalues.

We have used Algorithm 5.8 in a sample of 10^7 Markov matrices uniformly and independently distributed within the space Δ of 4×4 Markov matrices. As the set of Markov matrices might seem too general for

some applied problems (e.g. modeling the substitution of nucleotides in genomes), we have previously checked which of the matrices belonged to certain more restrictive families of matrices that appear in the literature. For instance, for Markov processes on (phylogenetic) trees it is important to restrict to matrices that are *diagonally largest in column* (DLC for short), i.e. Markov matrices whose diagonal entries are the largest entries in each column; see [7]. We denote this set of 4×4 Markov matrices by Δ_{dlc} . Usually, one can even restrict to the set Δ_{dd} of *diagonally dominant* matrices, that is, matrices $M \in \Delta$ satisfying $M_{ii} \geq 0.5$ for all i . If embeddable, these matrices have identifiable rates ([9]). Note that if a matrix is diagonally dominant, then its off-diagonal entries are smaller than or equal to 0.5. Hence, $\Delta_{\text{dd}} \subseteq \Delta_{\text{dlc}} \subseteq \Delta$. From a mathematical perspective, it makes sense to target the set of matrices that lie in the connected component of the identity matrix when we remove from Δ all matrices with determinant equal to 0. This set is called Δ_{Id} , corresponds to matrices with a positive determinant, and contains all embeddable Markov matrices.

	Samples	Embeddable samples	Percentage of embeddable
Δ	10^7	5774	0.05774
Δ_{Id}	4998008	5774	0.11553
Δ_{dlc}	148375	5460	3.67987
Δ_{dd}	2479	299	12.06132

TABLE 3. Based on a sample of 10^7 Markov matrices, the first column shows how many sample points lie in each set, the second column shows how many of them are embeddable, and the third column displays the corresponding percentage. Embeddability was checked with Algorithm 5.8.

Therefore, for each matrix generated, we have checked whether it belonged to each of the sets described above (Δ_{dlc} , Δ_{dd} , Δ_{Id}) and, by applying Algorithm 5.8, we have tested its embeddability. The results are shown in Table 3. To conclude, we would like to emphasize that, as the table shows, the percentage of embeddable Markov matrices is surprisingly small. This result should be taken as a warning signal as it probably has practical consequences related to modeling issues. Indeed, it may be advisable to reconsider the restriction and use of continuous-time homogeneous models, which seem to be very constrained even for DLC matrices.

Appendix A

In this appendix, we explain how to find generators for 4×4 Markov matrices with two repeated eigenvalues by using Algorithm 5.16. More

precisely, we explain how to check whether the intersection $\mathcal{P}_k \cap \mathcal{V}_+$ in Algorithm 5.16 is empty or not and how to choose a point in it (if not empty).

Let M be a diagonalizable 4×4 Markov matrix with a repeated eigenvalue and positive determinant, that is, $M = P \operatorname{diag}(1, \lambda, \mu, \mu)P^{-1}$ for some $P \in GL_4(\mathbb{R})$, $\lambda > 0$, and $\mu \in [-1, 1)$ such that $\mu \neq 0$ and $\mu \neq \lambda$. In this case, Theorem 5.11 yields that each Markov generator other than $\operatorname{Log}(M)$ can be uniquely expressed as $Q_k(x, y, z)$ for some $k \in \mathbb{Z}$ and some $(x, y, z) \in \mathcal{P}_k \cap \mathcal{V}_+$.

Assume that $k = 0$ and $\operatorname{Arg}(\mu) = 0$. Then, $Q_0(x, y, z)$ is equal to the principal logarithm of M for all (x, y, z) . Therefore, if the intersection $\mathcal{P}_k \cap \mathcal{V}_+$ is not empty, it is equal to \mathcal{V}_+ . In this case, the algorithm can choose any point $(x, y, z) \in \mathcal{V}_+$ such as $(1, 0, 1)$. For the remainder of this section we assume that $Q_k(x, y, z) \neq \operatorname{Log}(M)$. This assumption is equivalent to assuming that $2\pi k + \operatorname{Arg}(\mu) \neq 0$.

We denote by $l_{i,j}$ the entries of the matrix L in Definition 5.9 and by $p_{i,j}$ and $\tilde{p}_{i,j}$ the entries of P and P^{-1} respectively. \mathcal{P}_k is the set of solutions to the system of inequalities $Q_k(x, y, z)_{i,j} \geq 0$ for all $i \neq j$, where $Q_k(x, y, z) = L + (2\pi k + \operatorname{Arg}(\mu))V(x, y, z)$. A direct computation shows that the entries of $V(x, y, z)$ depend linearly on x, y , and z :

$$V(x, y, z)_{i,j} = p_{i,3}\tilde{p}_{4,j}x - p_{i,4}\tilde{p}_{3,j}z + (p_{i,4}\tilde{p}_{4,j} - p_{i,3}\tilde{p}_{3,j})y.$$

Hence, the planes $H_{i,j}$ containing the faces of \mathcal{P}_k are given by the equations:

$$(A.1) \quad p_{i,3}\tilde{p}_{4,j}x - p_{i,4}\tilde{p}_{3,j}z + (p_{i,4}\tilde{p}_{4,j} - p_{i,3}\tilde{p}_{3,j})y = \frac{-l_{i,j}}{2\pi k + \operatorname{Arg}(\mu)}.$$

From (A.1) we get that, for each $i \neq j$, the faces of two polyhedra \mathcal{P}_{k_1} and \mathcal{P}_{k_2} ($k_1, k_2 \in \mathbb{Z}$) corresponding to the (i, j) -entry of $Q_k(x, y, z)$ are necessarily parallel.

Let us define $f(x, y, z) = xz - y^2 - 1$ so that $\mathcal{V} = \{(x, y, z) \in \mathbb{R}^3 \mid f(x, y, z) = 0\}$. Note that $(x, y, z) \in \mathcal{V}_+$ if and only if $f(x, y, z) = 0$ and $x, z > 0$. Next we show how to find points in $\mathcal{P}_k \cap \mathcal{V}_+$. To do so, we evaluate $f(x, y, z)$ at the vertices, on edges and on faces of \mathcal{P}_k according to the following procedure:

Step 1. Evaluate $f(x, y, z)$ at each of the vertices of \mathcal{P}_k .

- If there is a pair of vertices v_1 and v_2 such that $f(v_1)f(v_2) < 0$, then \mathcal{V}_+ cuts \mathcal{P}_k and hence there are infinitely many generators. To find one of them, we restrict f to the line defined by v_1 and v_2 , and find a point $P = (x, y, z)$ in the segment between v_1 and v_2 such that $f(P) = 0$.

- If there is not such a pair of vertices but there is some vertex v satisfying $f(v) = 0$, then we take $P = v$.
- If the evaluation of f at all the vertices of \mathcal{P}_k has the same sign (and none is equal to 0), then we proceed to Step 2.

Step 2. Find the vanishing points of $f(x, y, z)$ on the edges of \mathcal{P}_k . To do so, we restrict f to the lines containing these edges and look for solutions $P = (x, y, z)$ of $f = 0$ lying on the corresponding edge.

- If we find two solutions in such a line, \mathcal{V}_+ cuts the interior of \mathcal{P}_k and hence there are infinitely many generators.
- If the edges of \mathcal{P}_k do not intersect \mathcal{V}_+ , then we proceed to Step 3.

Step 3. We assume that \mathcal{V} does not intersect any edge of \mathcal{P}_k . For $i \neq j$ consider the intersection $H_{i,j} \cap \mathcal{V}_+$, where $H_{i,j}$ is the plane defined by (A.1).

If this intersection is not empty, choose a point in it (see next paragraph) and check whether it belongs to \mathcal{P}_k or not. This intersection lies either completely in the corresponding face of the polyhedron or completely outside the polyhedron.

- If we find a point $P = (x, y, z)$ which belongs to the polyhedron in this way, then M has infinitely many generators and $Q_k(x, y, z)$ is one of them.
- If we fail to find a point in any of the faces, then M has no generator with the current value of k .

To conclude, we give some insight on how to find $P \in H_{i,j} \cap \mathcal{V}_+$ (when this intersection is not empty). For ease of reading we write $Ax + By + Cz = D$ for the equation of $H_{i,j}$ (see (A.1) for the precise coefficients). Given $(x, y, z) \in \mathcal{V}$, we can write $z = \frac{1+y^2}{x}$ because $x \neq 0$. Therefore, by multiplying the equation $Ax + By + Cz = D$ by x and rearranging the terms in the equality, we conclude that

$$Cy^2 + (Bx)y + (Ax^2 - Dx + C) = 0 \text{ if and only if } \left(x, y, \frac{1+y^2}{x}\right) \in \mathcal{V} \cap H_{i,j}.$$

Hence, $\mathcal{V}_+ \cap H_{i,j}$ is not empty if there exists $x > 0$ for which the discriminant

$$\Delta(x) := (B^2 - 4AC)x^2 + (4CD)x - 4C^2$$

is non-negative. We study below whether this is possible depending on the coefficients of $\Delta(x)$:

- (i) If $B^2 - 4AC < 0$, compute the roots of $\Delta(x) = 0$. If they are non-real or negative, then $\mathcal{V}_+ \cap H_{i,j} = \emptyset$. If both roots are real and positive, then all values between them satisfy $\Delta(x) \geq 0$. Note that in this case both roots have necessarily the same sign (because $\mathcal{V} \cap \{x = 0\} = \emptyset$).
- (ii) If $B^2 - 4AC > 0$, then $\Delta(x) > 0$ when $x \gg 0$.
- (iii) If $B^2 - 4AC = 0$ and $CD > 0$, then $\Delta(x) > 0$ when $x \gg 0$.
- (iv) If $B^2 - 4AC = 0$, $CD \leq 0$, and $C \neq 0$, then $\Delta(x) < 0$ for all $x \geq 0$. In this case, we have $\mathcal{V}_+ \cap H_{i,j} = \emptyset$.
- (v) If $\Delta(x)$ is identically 0, then $H_{i,j} \cap \mathcal{V}_+$ is unbounded with respect to x , that is, for any $x_0 > 0$, there are points $P = (x_0, y, z) \in H_{i,j} \cap \mathcal{V}_+$.

Note that in cases (ii), (iii), and (v) we have that $\Delta(x) \geq 0$ when $x \gg 0$ and hence the set $H_{i,j} \cap \mathcal{V}_+$ is unbounded with respect to x . Therefore, if we know that the polyhedron \mathcal{P}_k is bounded, then the intersection of \mathcal{V}_+ with the face (i, j) is necessarily empty in any of these cases.

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