The embedding problem for Markov matrices

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A l'avi.

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CONTENTS

NOTATION AND CONVENTIONS

We shall use the following notation throughout this work:

$M_n(\mathbb{C})$	space of $n \times n$ complex matrices
Id_n	identity matrix of size n
$J_m(\lambda)$	Jordan block of size m and eigenvalue λ
$\mathrm{Comm}^*(A)$	set of non-singular matrices that commute with A
$\mathrm{Arg}(\lambda)$	principal argument of $\lambda \in \mathbb{C}$
$\log_k(\lambda)$	k-th branch of the logarithm of $\lambda \in \mathbb{C} \setminus \{0\}$
$\log(\lambda)$	principal logarithm of $\lambda \in \mathbb{C} \setminus \{0\}$
$\mathrm{Log}(M)$	principal logarithm of a non-singular matrix M

All the matrices in this work are assumed to be square. We use eigenvector to denote right eigenvectors. Otherwise we will make explicit that we refer to left eigenvalues.

INTRODUCTION

Markov processes are stochastic processes in which the future is independent of the past, given the present. In this framework, Markov matrices are used to describe the changes of a discrete random variable over time. More precisely, *Markov matrices* (or *transition matrices*) are non-negative real square matrices with rows summing to one whose entries are the conditional probabilities of substitution between the states of a discrete random variable. When the probabilities of substitution are considered to be continuous (and differentiable) functions depending on time, Markov processes can be described in terms of the instantaneous rates of substitution between states. In order to keep such a process tractable, the substitution rates are usually assumed to be constant over time. In this case, we say that the process is a *homogeneous* continuous-time process and one displays all the rates together in a matrix called *rate matrix*. Rate matrices are real square matrices with rows summing to zero and non-negative off-diagonal entries. In this setting, given the rate matrix Q of the process, the transition matrix encoding the substitution probabilities after time t can be written as $M(t) = \exp(Qt)$. Any Markov matrix that can be written in this way is said to be "embeddable" because it can be embedded into the *Markov semigroup* $\{\exp(Qt),\ t \geq 0\}$. Equivalently, a Markov matrix M is *embeddable* if it can be written as the exponential of a rate matrix Q, $M = \exp(Q)$ (with no reference to time). In this case, any rate matrix Q satisfying $M = \exp(Q)$ is called a *Markov generator of M*. It is clear that not all Markov matrices are embeddable since a necessary condition for this is that the matrix is non-singular.

Question 1 (*Embedding problem* [Elf37])**:** Decide whether a given $n \times n$ Markov matrix is embeddable.

Solving the embedding problem results in giving necessary and sufficient conditions for a Markov matrix M to be embeddable. The characterization of 2×2 embeddable matrices was given by Kingman in [Kin62]. According to this solution, a 2×2 Markov matrix is embeddable if and only if its determinant is positive. Therefore, in this case one can easily decide whether a Markov matrix is embeddable without needing to compute any matrix logarithm. However, Kingman claimed that this did not seem feasible for Markov matrices of larger sizes. Actually, he even claimed that it seemed unlikely to obtain an explicit characterization for the embeddability of larger matrices (see [Dav10]).

The complete solution to the embedding problem for 3×3 matrices was not obtained until recently (see [CC11]). The characterization of embeddability in this case is much more cumbersome than in the case of 2×2 matrices, showing that Kingman was not completly wrong. Indeed, the solution is split into different cases depending on the Jordan decomposition of the Markov matrix and the full explicit solution has taken almost fourty years to be complete (see the contributions in [Cut73, Joh74, Car95, CC11]).

In addition to the solutions for 2×2 and 3×3 matrices, there are also several results regarding the embeddability of $n \times n$ matrices. Some of these involve necessary conditions in terms of the eigenvalues of the transition matrix [Elf37, Kin62, Run62] or sufficient conditions expressed in terms of the determinant of the Markov matrix [Cut73, Dav10, Goo70] or its entries [Fug88].

Besides asking for a criterion for embeddability, it is natural also to ask for conditions that guarantee the existence of a *unique* Markov generator. While the embedding problem is concerned with the existence of Markov generators, the rate identifiability problem focuses on their uniqueness. We say that an embeddable matrix has *identifiable rates* when there is only one Markov generator for it. There are several examples in the literature showing embeddable matrices that admit more than one Markov generator (see for example [Spe67, SS76, Dav10]).

Question 2 (Rate identifiability)**:** Characterize the $n \times n$ embeddable matrices that admit a unique Markov generator.

There are some known conditions that guarantee that the principal logarithm of a Markov matrix is its only real logarithm with rows summing to zero (see some examples in [Cut72, SS76, IRW01]). This leads to a number of partial solutions to the embedding problem which consist on checking whether the principal logarithm is a rate matrix or not. Actually, up to our knowledge, all the examples of embeddable matrices without repeated eigenvalues known before the results presented in this work (including those without identifiable rates) satisfy that their principal logarithm is a rate matrix.

Question 3: Is the embeddability of Markov matrices *with different eigenvalues* characterized by its principal logarithm?

Although the embedding problem is essentially a theoretical problem, it has been studied in detail in many applied areas due to its practical consequences. For example, in economic sciences by [IRW01, GMZ86], in social sciences (see [SS76]) and in evolutionary biology (e.g.[VYP$^+$13, Jia16, KK17, BS20]). Our original interest on the embedding problem arises from phylogenetics (the study of evolutionary relationships), where the embedding problem appears related to fundamental questions concerning the consistency of nucleotide substitution models. These models generally use a Markov process to describe the substitution of nucleotides over time in a given DNA sequence. The state space of the random variables in such a process consists on the four nucleotides in the DNA: adenine, guanine, cytosine and thymine.

The traditional approach to nucleotide substitution models is to consider homogeneous continuous-time Markov processes (see the first models in [JC69, Kim81, Fel81, Tav86]). Although real evolutionary processes are not homogeneous in general (see [HPCD05], for example), any substitution process in continuous-time can be approximated by concatenating short homogeneous processes. In this case, the transition matrix for the whole process is obtained by multiplying the (embeddable) transition matrices of the concatenated processes. If the resulting transition matrix is embeddable, then the original process can be modelled as homogeneous. However, the product of embeddable matrices is not necessarily an embeddable matrix.

Therefore, although the transition matrices of homogeneous continuous-time nucleotide substitution models are embeddable by construction, one still has to take the embedding problem into consideration in this framework.

An alternative approach to nucleotide substitution models is to avoid the time consideration and simply use a Markov matrix to rule the whole substitution process. This is a more general framework than that of homogeneous continuous-time, as it takes into account *all* Markov matrices, regardless of whether they are embeddable not. In contrast, some of the considered transition matrices can be argued to describe unrealistic evolutionary processes (e.g. permutation matrices). In this setting, the parameters of the model are the substitution probabilities (instead of the instantaneous rates of mutation). This approach has been used to study the geometric properties of the models with tools from algebraic geometry and commutative algebra (see [SS05, AR07, AR08, DK09]), which in turn has led to several algebraic methods for reconstructing the evolutionary history of living species without needing to estimate the substitution parameters (see for example the work in [Eri05, CFS07, RH12, CK14, AKR17]). Of course, these methods can be used for phylogenetic inference in the context of homogeneous continuous-time substitution processes. Actually, there are other reconstruction methods with an algebraic basis which have been explicitly defined for homogeneous continuous-time models (see [SCJJ08, HJS13]).

The connection between the two different frameworks for nucleotide substitution processes introduced above is intimately related to the embedding problem, as some Markov matrices are rejected or potentially considered depending on the approach.

Question 4: Quantify how many nucleotide transition matrices are consistent with a homogeneous continuous-time approach (i.e. are embeddable).

Depending on the approach, the assumptions of the *nucleotide substitution models* are expressed as constraints either in terms of the instantaneous rates of mutation or in terms of the substitution probabilities. These restrictions are usually motivated by observations on the frequencies of substitutions between nucleotides (see [Kim80, Kim81]) or by mathematical convenience (e.g. [Fel04, Tav86]). A natural question is that of deciding when a transition matrix subject to model constraints admits a Markov generator with the same restrictions on its entries (*model-embeddability*).

Question 5: Quantify the proportion of both embeddable and model-embeddable transition matrices within a particular nucleotide substitution model.

Throughout this memoir we give answers to the problems above and to other related questions. Next, we outline the structure and the main results of this report.

In Chapter 1 we introduce the basic definitions and results that shall be used throughout this work and we give a detailed background on the embedding problem. We also introduce there the description of all matrix logarithms (real or not) detailed in [Gan59] and the characterization of matrices with real logarithms due to Culver [Cul66], which are fundamental for most of our contributions. In the last section of Chapter 1, we focus on nucleotide substitution models and the impact of the embeding problem in this framework. In particular, we give evidence that all embeddable nucleotide transition matrices are biologically meaningful (see Remark 1.4.13).

In Chapter 2 we study the embeddability and rate identifiability of Markov matrices of any size (Questions 1 and 2). We give tighter bounds on the eigenvalues of rate matrices than already existing ones. Based on this, we give a sufficient condition for the embeddability of Markov matrices that relaxes the hypothesis of similar known results (cf. [Cut73, IRW01]).

Theorem 1 (Theorem 2.2.5)**.** *Let M be an $n \times n$ diagonalizable Markov matrix and let Λ be the set formed by its non-real eigenvalues and its eigenvalues with multiplicity ≥ 2. Then, the unique possible Markov generator of M is $\mathrm{Log}(M)$ if for all $z \in \Lambda$ we have $\beta_n(z) \leq \pi$, where*

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

In this case, M is embeddable if and only if $\mathrm{Log}(M)$ *is a rate matrix.*

In addition to this partial solution to the embedding problem (and also to the rate identifiabily problem), we give a criterion to test the embeddability of any $n \times n$ Markov matrix with different eigenvalues:

Theorem 2 (Theorem 2.3.3)**.** *Let M be a Markov matrix with an eigen-decomposition of the form*

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

with $P \in GL_n(\mathbb{C})$, $\lambda_i \in (0,1)$ for $i = 1, \dots, t$, $\mu_j \in \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$ for $j = 1, \dots, s$, all of them pairwise different. Let $\log_k(\mu)$ denote the $k-th$ branch of the logarithm of μ. Then, M is embeddable if and only if

$$P\ \mathrm{diag}\Big(0, \log(\lambda_1), \dots, \log(\lambda_t), \log_{k_1}(\mu_1), \overline{\log_{k_1}(\mu_1)}, \dots, \log_{k_s}(\mu_s), \overline{\log_{k_s}(\mu_s)}\Big)\ P^{-1}$$

is a rate matrix for some $k_1, \dots, k_s \in \mathbb{Z}^s$ satisfying

$$\left\lceil \tfrac{-\mathrm{Arg}(\mu_j) - \beta_n(\mu_j)}{2\pi} \right\rceil \leq k_j \leq \left\lfloor \tfrac{-\mathrm{Arg}(\mu_j) + \beta_n(\mu_j)}{2\pi} \right\rfloor .$$

Using this, we get an algorithm that can be used to find all the Markov generators of any given Markov matrix with different eigenvalues (Algorithm 2.3.5). In particular, this algorithm solves both the embedding problem and and the rate identifiability problem for a dense subset of $n \times n$ Markov matrices for any $n \in \mathbb{N}$.

In Chapter 3 we focus on the embedding problem and the rate identifiability problem for 4×4 Markov matrices. As in the case of 3×3 Markov matrices, our proposed solution to these problems is split into several results depending on the Jordan form of the given Markov matrix (see Table 3.2). The particular case of Markov matrices with different eigenvalues is solved by specializing the results in the previous chapter to 4×4 matrices, which results in an explicit criterion for both embeddability and rate identifiability in this case .

Theorem 3 (Theorem 3.2.1)**.** *Let $M = P\mathrm{diag}(1, \lambda_1, \lambda_2, \lambda_3)P^{-1}$ 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* $V = P\,\mathrm{diag}(0, 0, 2\pi i, -2\pi i)\,P^{-1}$ *and*

$$\mathcal{L} := \max_{(i,j):\ i\neq j,\ V_{i,j}>0} \left\lceil -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rceil, \quad \mathcal{U} := \min_{(i,j):\ i\neq j,\ V_{i,j}<0} \left\lfloor -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rfloor.$$

Otherwise, write $\mathcal{L} = \mathcal{U} = 0$ *and let* V *denote the* 4×4 *zero matrix. Set*

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

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* $\mathrm{Log}(M) + kV$ *with* $k \in [\mathcal{L}, \mathcal{U}]$.

In addition, we provide an algorithm to test the embeddability of Markov matrices with an eigenvalue with multiplicity 2 (Algorithm 3.2.3) and another algorithm to test the embeddability of the remaining Markov matrices (Algorithm 3.2.2). By applying this last algorithm on a uniformly generated random sample of Markov matrices with different eigenvalues, we are able to estimate the proportion of embeddable matrices within the set of 4×4 Markov matrices (Question 4). According to the results obtained, only about a 0.05% of 4×4 Markov matrices are embeddable (see Table 3.1).

In Chapter 4 we solve the embedding problem for the Kimura 3-parameter model [Kim81] and its submodels, the Kimura 2-parameter model [Kim80] and the Jukes-Cantor model [JC69]. The following theorem summarizes the related results and gives a criterion to test the embeddability of generic Kimura 3-parameter Markov matrices.

Theorem 4 (see Proposition 3.1.14 and Corollaries 4.2.1 and 4.2.6)**.** *Let* M *be a Kimura 3-parameter Markov matrix with eigenvalues* $1, \lambda, \mu, \gamma$. *Then, if* M *has no repeated negative eigenvalue, the following are equivalent:*

i) M *is embeddable.*

ii) M *is model-embeddable.*

iii) The principal logarithm of M *is a rate matrix.*

iv) The eigenvalues of M are strictly positive and satisfy

$$\lambda \geq \mu\gamma, \qquad \mu \geq \lambda\gamma, \qquad \gamma \geq \lambda\mu.$$

This result exhibits that the answer to Question 3 is affirmative when we restrict to the Kimura 3-parameter model or to any of its submodels. We also study the case of repeated eigenvalue in great detail. More precisely, we see that Kimura 3-parameter matrices with a repeated eigenvalues can be considered to belong to the Kimura 2-parameter model without loss of generality. In this context, we give a criterion for the embeddability and for the rate identifiability of generic Kimura 2-parameter matrices.

Theorem 5 (Theorem 4.3.8)**.** *For any given Kimura 2-parameter Markov matrix* $M = \begin{pmatrix} a & b & c & c \\ b & a & c & c \\ c & c & a & b \\ c & c & b & a \end{pmatrix}$ *with* $b \neq c$*, the following holds:*

a) If $c = 0.5 - b$*, then M is not embeddable.*

b) If $c < 0.5 - b$*, M is embeddable if and only if* $c \leq \sqrt{b} - b$*. In this case,*

- *i) If* $c < \frac{1-e^{-4\pi}}{4}$*, then the rates of M are identifiable.*
- *ii) If* $c = \frac{1-e^{-4\pi}}{4}$*, then M has exactly 3 Markov generators.*
- *iii) If* $c > \frac{1-e^{-4\pi}}{4}$*, then M has infinitely many Markov generators.*

c) If $c > 0.5 - b$*, M is embeddable if and only if* $\frac{1-e^{-2\pi}}{4} \leq c \leq \sqrt{b} - b$*. In this case the rates of M are not identifiable. Moreover,*

- *i) If* $c = \frac{1-e^{-2\pi}}{4}$*, then M has exactly 2 Markov generators.*
- *ii) If* $c > \frac{1-e^{-2\pi}}{4}$*, then M has infinitely many Markov generators.*

Unlike the case of generic Kimura 3-parameter matrices, we see that embeddable Kimura 2-parameter matrices may have unidentifiable rates. Moreover, we see that there are Kimura 2-parameter embeddable matrices that are not model-embeddable. This shows that rates may not be able to reproduce symmetric constraints among probabilities and seems to be inconsistent with the original approach of Kimura models via mutation rates, where the symmetries between transition and transversion probabilities are to be captured by the rate matrix [Kim80, Kim81].

In this chapter, we also compute the proportion of embeddable and model-embedable matrices within the Kimura 3-parameter model, the Kimura 2-parameter model and the Jukes-Cantor model (Question 5). We get that only a 9.375% of the transition matrices in the Kimura 3-Parameter model are embeddable, whereas for the Kimura 2-parameter model the proportion barely surpasses the 33%. Finally, the Jukes-Cantor model has a 75% of embeddable matrices.

In Chapter 5 we focus on the strand-symmetric model defined in [YP04, CS05]. We show that, under the assumption of different eigenvalues, the embeddability and model-embeddability of matrices within the strand symmetric model are equivalent (Proposition 5.1.2) and we give a necessary condition to guarantee both of them.

Theorem 6 (Theorem 5.1.8)**.** *Let M be a strand-symmetric Markov matrix with different eigenvalues. If M is embeddable, then one of the following does necessarily hold:*

i) $\mathrm{Log}(M)$ *is a rate matrix.*

ii) $\mathrm{Log}(M)$ *has no null entries and exactly two negative off-diagonal entries, which lie in its anti-diagonal.*

Although we do not provide an explicit criterion for the embeddability of strand-symmetric matrices, we can estimate the proportion of embeddable matrices within the model by applying algorithm 3.2.2 on a uniformly generated random sample of strand symmetric matrices. According to the results obtained, only about 1.75% of Markov matrices within the strand-symmetric model are embeddable (same for model-embeddable). We finish this chapter by constructing a family of examples within the strand-symmetric model to show that the answer to Question 3 can be negative (see Examples 5.2.4 and 5.2.5). Moreover, we are able to perturb these examples to prove that it is *generically* false that the embeddability of 4×4 Markov matrices is determined by its principal logarithm.

Theorem 7 (see Theorem 5.3.1)**.** *There is an Euclidean open set of embeddable Markov matrices whose principal logarithm is not a Markov generator within the set of* 4×4 *Markov matrices.*

We conclude the introduction by summarizing the results obtained for Question 5 for the different nucleotide substitution models considered in Chapters 3, 4 and 5. We note that the simpler the model is, the larger the proportion of embeddable matrices within the model.

Model	**Proportion of embeddable**
General Markov	0.00057
Strand symmetric	0.0175
Kimura 3-parameter	0.09375
Kimura 2-parameter	0.33336
Jukes-Cantor	0.75

PUBLICATIONS

The results obtained in this thesis are part of the following research articles:

- Roca-Lacostena, J. Generating embeddable matrices whose principal logarithm is not a Markov generator. To appear in *Trends in Mathematics, Research Perspectives CRM Barcelona*, vol. 12. Birkhäuser.

- Casanellas, M., Fernández-Sánchez, J., and Roca-Lacostena, J. (2020). An open set of 4×4 embeddable matrices whose principal logarithm is not a Markov generator. *Linear and Multilinear Algebra*, vol. 0(0), pp. 1–12.

- Casanellas, M., Fernández-Sánchez, J., and Roca-Lacostena, J. (2020). The embedding problem for Markov matrices. arXiv: 2005.00818 [math.PR].

- Casanellas, M., Fernández-Sánchez, J., and Roca-Lacostena, J. (2020). Embeddability and rate identifiability of Kimura 2-parameter matrices. *Journal of Mathematical Biology*, vol. 80, pp. 995–1019.

- Roca-Lacostena, J. and Fernández-Sánchez, J. (2018). Embeddability of Kimura 3ST Markov matrices. *Journal of Theoretical Biology*, vol. 445, pp. 128 – 135.

1

PRELIMINARIES

In this chapter we introduce the definitions and results that will be used throughout this thesis. The chapter is divided into four sections. In the first section we explain how to apply real and complex functions to matrices. We focus on the matrix exponential and the matrix logarithm as they are required to state the embedding problem.

In the second section we recall some known results about Markov processes and introduce Markov matrices and rate matrices as well as some of their properties. The contents in this section motivate the *embedding problem* for Markov matrices [Elf37].

In the third section, we talk about the existence and uniqueness of solutions to the embedding problem. More precisely, we give a survey on the solutions to this problem for the cases that had been already solved (that is 2×2 and 3×3 matrices) and we also present some known results for the general case. The uniqueness of solutions to the embedding problem is discussed in the framework of the *rate identifiability problem*, which is introduced in this section.

Finally, in the fourth section we introduce nucleotide substitution models, which motivated the present work. Markov matrices of size four play a special role in this case, as they are used as the transition matrices of the underlying Markov processes. We discuss the consequences (in terms of modelling) of restricting to embeddable matrices in this context.

All the results in this chapter of the memoir are known results which can be found in the literature. We include some proofs for completeness,in particular we give the proofs that we have worked out which, in some cases, are original and different from the ones presented in the references.

1.1 FUNCTIONS OF MATRICES

In this section we explain how to extend complex functions to square matrices. Almost all the results in this section are well-known and can be found in most books on linear algebras, such as [Gan59] and [Mey00], or in more specific volumes like [Hig08]. Throughout this work we shall only consider square matrices and use the following notation (see also the notation list in page 9).

Notation. $M_n(\mathbb{K})$ denotes the set of $n \times n$ square matrices with entries in a field $\mathbb{K}$ and we shall only consider $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. $GL_n(\mathbb{K})$ is the subset of non-singular matrices in $M_n(\mathbb{K})$. We denote the identity matrix of size n as Id_n (or simply Id when the size is understood form the context) and we use $\mathbf{1}$ to refer to the vector $(1, \ldots, 1)^t$. We use the word *eigenvector* to denote right eigenvectors and we refer to left-eigenvectors explicitly. The set of all eigenvalues of a matrix $A \in M_n(\mathbb{K})$ is the *spectrum of* A and is denoted by $\sigma(A)$. We denote by a_λ the *algebraic multiplicity* of the eigenvalue λ and by g_λ its *geometric multiplicity* (that is, the dimension of $\mathrm{Ker}(A - \lambda Id_n)$).

1.1.1 Jordan Decomposition

In this subsection we recall the Jordan decomposition of a matrix and state some of its properties. This will be used later in Section 1.1.4 to enumerate all the possible logarithms of any non-singular square matrix.

Definition 1.1.1. Given $A \in M_n(\mathbb{C})$, a matrix $J \in M_n(\mathbb{C})$ is a *Jordan canonical form* of A if there is a non-singular matrix P such that $P^{-1}\ A\ P = J$ and $J = \mathrm{diag}(J_{m_1}(\lambda_1), \ldots, J_{m_s}(\lambda_s))$ where $m_i \in \mathbb{N}$, $m_1 + \cdots + m_s = n$

and $J_m(\lambda)$ denotes the upper-triangular matrix

$$J_m(\lambda) := \begin{pmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix} \in M_m(\mathbb{C}).$$

A *Jordan decomposition* of A is a factorization of A into a Jordan canonical form:

$$A = P\,J\,P^{-1}. \tag{1.1}$$

It is well known that any matrix in $M_n(\mathbb{C})$ admits a Jordan decomposition and that the values λ_i above are the eigenvalues of A. We say that each $J_m(\lambda)$ is an $m \times m$ *Jordan block* of eigenvalue λ. In this case, we say that P is a *Jordan transformation matrix* for A. The Jordan canonical form of A, namely J, is unique up to the ordering of the Jordan blocks. However, even if we fix an ordering on these, the Jordan transformation matrix P is not unique.

The *Jordan segment* of eigenvalue λ is the $a_\lambda \times a_\lambda$ block-diagonal matrix containing all the Jordan blocks of eigenvalue λ, ordered by decreasing size, and is denoted by J_λ. The geometric multiplicity of λ, g_λ, coincides with the number of Jordan blocks in the Jordan segment J_λ. If all the eigenvalues of A have the same algebraic and geometric multiplicity then all the Jordan blocks in J have size 1 and $s = n$, thus $J = \operatorname{diag}(\lambda_1, \ldots, \lambda_s)$. In this case we say that A *diagonalizes* and a Jordan decomposition as in (1.1) is also called an *eigendecomposition* of A.

Example 1.1.2. Consider the following matrices

$$A = \frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & 3 & 1 \\ 0 & -2 & 0 & 0 & 0 \\ -2 & 6 & -1 & -3 & 5 \\ 4 & 0 & 1 & 1 & -1 \\ 0 & 6 & 0 & 0 & 4 \end{pmatrix} \qquad P = \begin{pmatrix} 1 & -1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix}.$$

A straightforward computation shows that P is a Jordan transformation matrix for A. Indeed,

$$J = P^{-1}\, A\, P = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

is a Jordan form of A formed by four Jordan blocks. The spectrum of A is $\sigma(A) = \{-1, 2\}$. The algebraic multiplicity of -1 is $a_{-1} = 3$ and its geometric multiplicity is $g_{-1} = 2$. As mentioned above, the algebraic multiplicity coincides with the size of the corresponding Jordan segment whereas the geometric multiplicity is the number of Jordan blocks in it, so

$$J_1 = \mathrm{diag}(J_2(1), J_1(1)) = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

On the other hand, $a_2 = 2$ and $g_2 = 2$. Since $a_2 = g_2$, the Jordan segment with eigenvalue 2 is the diagonal matrix

$$J_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}.$$

Next we show how to obtain all the Jordan transformation matrices from a given one. To this aim we first introduce the commutant of a matrix.

Definition 1.1.3. Given a square matrix M, the *commutant group* of M is the set of invertible complex matrices that commute with M:

$$\mathrm{Comm}^*(M) = \{N \in GL_n(\mathbb{C}) : MN = NM\}.$$

Lemma 1.1.4. *Given a matrix A, let $P\, J\, P^{-1}$ be a Jordan decomposition of A. Then the set of all Jordan transformation matrices for A is*

$$\{\widetilde{P} = PC : C \in \mathrm{Comm}^*(J)\}.$$

Proof. If $C \in \mathrm{Comm}^*(J)$, then $(PC)J(PC)^{-1} = PJP^{-1} = A$ thus PC is a Jordan transformation matrix. Conversely, given P and $\widetilde{P}$ two Jordan transformation matrices for A we have $\widetilde{P}J\widetilde{P}^{-1} = A = PJP^{-1}$. Hence $(P^{-1}\widetilde{P})J = J(P^{-1}\widetilde{P})$, so $C := P^{-1}\,\widetilde{P}$ belongs to $\mathrm{Comm}^*(J)$. □

The next proposition gives a description of the commutant of a matrix in Jordan form and also shows that it does not depend on the eigenvalues but on the structure of the Jordan blocks.

Proposition 1.1.5. *The following holds:*

i) $\mathrm{Comm}^*(\lambda Id_n) = GL_n(\mathbb{C})$ *for any* $\lambda \in \mathbb{C}$.

ii) If $J_{\lambda_1}, \dots, J_{\lambda_s}$ *are Jordan segments with different eigenvalues, then*

$$\mathrm{Comm}^*(\mathrm{diag}(J_{\lambda_1}, \dots, J_{\lambda_s})) = \{\mathrm{diag}(C_1, \dots, C_s) : C_i \in \mathrm{Comm}^*(J_{\lambda_i})\}.$$

iii) If J_{λ_1} *and* J_{λ_2} *are two Jordan segments with the same block structure then* $\mathrm{Comm}^*(J_{\lambda_1}) = \mathrm{Comm}^*(J_{\lambda_2})$.

Proof.

i) This is immediate because λId_n commutes with any matrix in $M_n(\mathbb{C})$.

ii) Let us write $J = \mathrm{diag}(J_{\lambda_1}, \dots, J_{\lambda_s})$. We prove both inclusions:

$\supseteq$) This inclusion follows immediately by block multiplication.

$\subseteq$) Given $C \in \mathrm{Comm}^*(J)$, let us split it into blocks as:

$$C = \begin{pmatrix} C_{1,1} & \dots & C_{1,s} \\ \vdots & \ddots & \vdots \\ C_{s,1} & \dots & C_{s,s} \end{pmatrix} \text{ with } C_{i,i} \in M_{a_{\lambda_i}}(\mathbb{C}).$$

As $JC - CJ = 0$ we get $J_{\lambda_i}C_{i,j} - C_{i,j}J_{\lambda_j} = 0$ for all i, j. Thus, for $i = j$ this implies that $C_{i,i} \in \mathrm{Comm}^*(J_{\lambda_i})$. In order to conclude the proof we want to see that, if $i \neq j$, then $C_{i,j} = 0$. For indices

i and j such that $i \neq j$, we write $A = J_{\lambda_i}$, $B = J_{\lambda_j}$ and $E = C_{i,j}$. Then,

$$(AE)_{k,l} = \begin{cases} \lambda_i E_{k,l} + E_{k+1,l} & \text{if } A_{k,k+1} = 1, \\ \lambda_i E_{k,l} & \text{if } k = a_{\lambda_i} \text{ or } A_{k,k+1} = 0 \end{cases}$$

and

$$(EB)_{k,l} = \begin{cases} \lambda_j E_{k,l} + E_{k,l-1} & \text{if } B_{k,l-1} = 1, \\ \lambda_j E_{k,l} & \text{if } l = 1 \text{ or } B_{k,l-1} = 0. \end{cases}.$$

Since the Jordan segment J_{λ_i} includes all Jordan blocks with eigenvalue λ_i we have $\lambda_i \neq \lambda_j$. Hence, $AE - EB = 0$ implies that $E_{k,l} = 0$ for all k, l and also that $C_{i,j} = 0$ for $i \neq j$.

iii) If J_{λ_1} and J_{λ_2} have the same Jordan block structure, then $J_{\lambda_1} - J_{\lambda_2} = (\lambda_1 - \lambda_2)Id$. In this case, for any $C \in \text{Comm}^*(J_{\lambda_1})$ we have:

$$C\ J_{\lambda_1} - C\ J_{\lambda_2} = C\big((\lambda_1 - \lambda_2)\ Id\big) = \big((\lambda_1 - \lambda_2)\ Id\big)\ C = J_{\lambda_1}\ C - J_{\lambda_2}\ C.$$

Hence, $C\ J_{\lambda_2} - J_{\lambda_2}\ C = C\ J_{\lambda_1} - J_{\lambda_1}\ C = 0$ and hence $\text{Comm}^*(J_{\lambda_1}) \subseteq \text{Comm}^*(J_{\lambda_2})$. The opposite inclusion follows by symmetry. □

1.1.2 Spectral Resolution of a function

Throughout this report we shall be working with functions of matrices defined the via spectral resolution or via a power series. The first approach is based on applying a well-defined function and its successive derivatives to the eigenvalues of the matrix via its Jordan canonical form, whereas the second approach consists on applying the Taylor series of the function to the matrix. It is known that, when both methods can be applied, the resulting matrices are equal [Hig08, Section 1.2]. Besides these, there are other equivalent approaches based on the Hermite interpolation polynomial or the Cauchy integral (see [Hig08, Chap.1] for details).

Definition 1.1.6. Given $A \in M_m(\mathbb{C})$ with spectrum $\sigma(A) = \{\lambda_1, \ldots, \lambda_s\}$, let ι_i denote the maximum size of the Jordan blocks of eigenvalue λ_i. A complex-valued function f is said to be *defined on the spectrum* of A if the successive derivatives $f^{(j)}(\lambda_i)$ are defined for each $j = 0, \ldots, \iota_i - 1$, $i \in \{1, \ldots, s\}$.

Definition 1.1.7. Given $A \in M_m(\mathbb{C})$, let $J = \mathrm{diag}(J_{m_1}(\lambda_1), \ldots, J_{m_s}(\lambda_m))$ be its Jordan canonical form. Given a function f defined on the spectrum of A, we define the *spectral resolution of f in A* as

$$f(A) = P\mathrm{diag}(f(J_{m_1}(\lambda_1)), \ldots, f(J_{m_s}(\lambda_s)))P^{-1},$$

where

$$f(J_{m_k}(\lambda_k)) = \begin{pmatrix} f(\lambda_k) & f'(\lambda_k) & \cdots & \frac{f^{m_k-1}(\lambda_k)}{(m_k-1)!} \\ & f(\lambda_k) & \ddots & \vdots \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{pmatrix}, \text{ for } k = 1, \ldots, s.$$

Note that $f(A) = Pf(J)P^{-1}$. In the particular case that A diagonalizes with an eigendecomposition $P\ \mathrm{diag}(\lambda_1, \ldots, \lambda_s)\ P^{-1}$ we have that $f(A)$ also diagonalizes and

$$f(A) = P\ \mathrm{diag}(f(\lambda_1), \ldots, f(\lambda_s))\ P^{-1}.$$

Remark 1.1.8. If f is defined on the spectrum of a block-diagonal matrix $A = \mathrm{diag}(A_1, \ldots, A_s)$, then the spectral resolution of f in A can be computed block-wise. Indeed, f is defined on the spectrum of each block A_i, $i = 1, \ldots, s$. Since each block A_i admits a Jordan decomposition $A_i = P_i J_i P_i^{-1}$ we have that $\mathrm{diag}(J_1, \ldots, J_s)$ is a Jordan form of A and the corresponding transformation matrix is $P = \mathrm{diag}(P_1, \ldots, P_s)$ (note that the blocks in this Jordan form may appear in a different order than in Jordan form of A introduced in Definition 1.1.1). Therefore we have:

$$f(A) = \begin{pmatrix} P_1 & & \\ & \ddots & \\ & & P_s \end{pmatrix} \begin{pmatrix} f(J_1) & & \\ & \ddots & \\ & & f(J_s) \end{pmatrix} \begin{pmatrix} P_1^{-1} & & \\ & \ddots & \\ & & P_s^{-1} \end{pmatrix}.$$

Remark 1.1.9. The spectral resolution of a function f in a matrix A is well-defined in the sense that it does not depend on the transformation matrix P. If A diagonalizes this can be inferred from Lemma 1.1.4 together with Proposition 1.1.5. We refer to [Mey00, pp. 601-603] for a detailed proof in the case of non-diagonalizable matrices.

In general, it is not true that $f(J_m(\lambda)) = J_m(f(\lambda))$ for $m > 1$. Nonetheless, we have the following result.

Lemma 1.1.10. *If $f(\lambda), f'(\lambda), \ldots, f^{(m-1)}(\lambda)$ are defined for a complex-valued function f and $f'(\lambda) \neq 0$, then the Jordan form of $f(J_m(\lambda))$ is $J_m(f(\lambda))$.*

Proof. Note that $f(J_m(\lambda))$ has only one eigenvalue, namely $f(\lambda)$. Moreover, since $f'(\lambda) \neq 0$ we have that $\operatorname{rank}(f(J_m(\lambda)) - f(\lambda)Id) = m - 1$, so $\dim(\operatorname{Ker}(f(J_m(\lambda)) - f(\lambda)Id)) = 1$. Hence $f(\lambda)$ is an eigenvalue of $f(J_m(\lambda))$ with algebraic multiplicity m and geometric multiplicity 1. This guarantees the claim. □

1.1.3 Matrix exponential

Using the previous section one can define the exponential of a matrix A, $\exp(A)$, via the spectral resolution. However, one can also define it by applying the Taylor power series of $f(x) = e^x$ to the matrix, that is,

$$\exp(A) = \sum_{k=0}^{\infty} \frac{A^k}{k!}, \text{ where } A^0 = Id. \tag{1.2}$$

Since the power series above is absolutely convergent for any matrix and the exponential function is holomorphic in $\mathbb{C}$, both approaches to define the exponential of a matrix can be applied to any square matrix. Throughout this work we will use both methods indistinctly. We shall denote the exponential of a complex number x by e^x and the exponential of a matrix A by $\exp(A)$. In this subsection we state some properties of the exponential of a matrix.

Example 1.1.11. If we compute the exponential of a Jordan block $J(\lambda)$ via its spectral resolution we get

$$\exp(J_n(\lambda)) = \begin{pmatrix} e^\lambda & e^\lambda & \frac{e^\lambda}{2!} & \cdots & \frac{e^\lambda}{(n-1)!} \\ & e^\lambda & e^\lambda & \ddots & \vdots \\ & & \ddots & \ddots & \frac{e^\lambda}{2!} \\ & & & e^\lambda & e^\lambda \\ & & & & e^\lambda \end{pmatrix}.$$

Similarly, we can compute the exponential of a matrix A with Jordan decomposition $A = P\ J\ P^{-1}$, $J = \mathrm{diag}(J_{m_1}(\lambda_1), \ldots, J_{m_s}(\lambda_s))$, $P \in GL_n(\mathbb{C})$. In this case we have $\exp(A) = P\ \exp(J)\ P^{-1}$. More precisely,

$$\exp(A) = P\ \mathrm{diag}(\exp(J_{m_1}(\lambda_1)), \ldots, \exp(J_{m_s}(\lambda_s)))\ P^{-1}. \tag{1.3}$$

In particular, if A diagonalizes so does $\exp(A)$ and

$$\exp(P\ \mathrm{diag}(\lambda_1, \ldots, \lambda_n)\ P^{-1}) = P\ \mathrm{diag}(e^{\lambda_1}, \ldots, e^{\lambda_n})\ P^{-1}. \tag{1.4}$$

Note that $e^\lambda \neq 0$ for any $\lambda \in \mathbb{C}$, thus Lemma 1.1.10 applies and the Jordan form of $\exp(J_n(\lambda))$ is $J_n(e^\lambda)$. Analogously, $\mathrm{diag}(J_{m_1}(e^{\lambda}_1), \ldots, J_{m_s}(e^{\lambda}_s))$ is a Jordan form of $\exp(A)$.

Lemma 1.1.12. *If v is an eigenvector of a matrix A with eigenvalue λ, then v is an eigenvector of* $\exp(A)$ *with eigenvalue e^λ.*

Proof. Since v is an eigenvector of A, we have $\exp(A)\ v = \left(\sum_{k=0}^{\infty} \frac{A^k}{k!}\right)\ v = \sum_{k=0}^{\infty} \frac{A^k\ v}{k!} = \sum_{k=0}^{\infty} \frac{\lambda^k v}{k!} = e^\lambda\ v$. □

Remark 1.1.13. Note that the converse is not true in general. For instance, consider the matrix

$$A = \begin{pmatrix} 0 & 2\pi \\ -2\pi & 0 \end{pmatrix}$$

whose exponential is the identity matrix Id_2 (this is shown in the forthcoming Example 1.1.23). Note that $(1,0)^t$ is not an eigenvector of A but it is an eigenvector of $\exp(A)$.

Due to the non-commutativity nature of matrix multiplication it is generally false that $\exp(A)\exp(B) = \exp(A+B)$. However, if A and B commute this formula holds.

Proposition 1.1.14. *If $A, B \in M_n(\mathbb{C})$ commute then* $\exp(A+B) = \exp(A)\exp(B)$.

Proof. If A and B commute then we can apply the binomial theorem to compute $(A+B)^k$. Hence

$$\sum_{i=0}^{N} \frac{(A+B)^i}{i!} = \sum_{i=0}^{N}\sum_{j=0}^{i} \binom{i}{j} \frac{A^{i-j}B^j}{i!} = \sum_{i=0}^{N}\sum_{j=0}^{i} \frac{A^{i-j}}{(i-j)!}\frac{B^j}{j!}.$$

On the other hand,

$$\left(\sum_{k=0}^{N} \frac{A^k}{k!}\right)\left(\sum_{l=0}^{N} \frac{B^l}{l!}\right) = \sum_{k=0}^{N}\left(\frac{A^k}{k!}\sum_{l=0}^{N}\frac{B^l}{l!}\right) = \sum_{k=0}^{N}\sum_{l=0}^{N}\frac{A^k}{k!}\frac{B^l}{l!}.$$

By taking the limit when N tends to infinity in both expressions above we get

$$\exp(A+B) = \sum_{i=0}^{\infty}\sum_{j=0}^{i} \frac{A^{i-j}}{(i-j)!}\frac{B^j}{j!}$$

and

$$\exp(A)\exp(B) = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{A^k}{k!}\frac{B^l}{l!}.$$

Note that both sums converge because the exponential power series is convergent. Moreover, they are equal because we can set any values for i, j in the first series and see that the same term appears in the second expression, and vice versa. □

Remark 1.1.15. The Baker–Campbell–Hausdorff formula [Cam97] gives an explicit expression for $\exp(A+B)$, even if A and B do not commute. In particular, it shows that the converse of the previous proposition is also true.

We conclude this section by presenting another well-known result which relates the trace of a matrix and the determinant of its exponential.

Proposition 1.1.16. *For any matrix $A \in M_n(\mathbb{C})$ we have*

$$e^{\operatorname{tr}(A)} = \det(\exp(A)).$$

Proof. Let $J_A = \operatorname{diag}(J_{m_1}(\lambda_1), \dots, J_{m_s}(\lambda_s))$ be a Jordan canonical form of A. According to Lemma 1.1.10, $J_{\exp(A)} = \operatorname{diag}(J_{m_1}(e^{\lambda_1}), \dots, J_{m_s}(e^{\lambda_s}))$ is a Jordan canonical form of $\exp(A)$. Since both the trace and the determinant of a matrix are invariant under change of basis, we get $e^{\operatorname{tr}(A)} = e^{\operatorname{tr}(J_A)} = e^{m_1\lambda_1 + \cdots + m_s\lambda_s} = (e^{\lambda_1})^{m_1} \cdots (e^{\lambda_s})^{m_s} = \det(J_{\exp(A)}) = \det(\exp(A))$. □

1.1.4 Matrix logarithms

In this section we recall the definition of the logarithms of a matrix and explain how to find all of them.

Definition 1.1.17. Let A and L be in $M_n(\mathbb{C})$. L is said to be a *logarithm of* A if $\exp(L) = A$.

Remark 1.1.18. From Proposition 1.1.16 we get that $\det(\exp(L))$ is never 0. Thus, singular matrices have no logarithm.

It is known that the spectral resolution is consistent with function composition [Mey00, Ex. 7.9.18]. That is,

$$(f \circ g)(A) = f(g(A)) \tag{1.5}$$

provided that $g(A)$ and $f(g(A))$ are well-defined. Therefore, one can obtain matrix logarithms by using the spectral resolution of the logarithm function.

Example 1.1.19. Let us consider the following matrices:

$$A = \begin{pmatrix} 0.6 & 0.2 \\ 0.2 & 0.9 \end{pmatrix} \qquad P = \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}.$$

A direct computation shows that $P \operatorname{diag}(1, 0.5)\, P^{-1}$ is an eigendecomposition of A. Since the real logarithm function log is defined on the spectrum of A, $\sigma(A) = \{1, 0.5\}$, we can obtain a logarithm of A by computing the spectral resolution of log in A:

$$\log(A) = P\,\mathrm{diag}(\log(1), \log(0.5))\,P^{-1} \approx \begin{pmatrix} -0.5545177445 & 0.2772588722 \\ 0.2772588722 & -0.138694361 \end{pmatrix}.$$

Indeed, we have $\exp(\log(A)) = (\exp \circ \log)(A) = A$ by (1.5).

However, if one is interested in computing all the logarithms of a matrix then all branches of the complex logarithm have to be considered. Indeed, a different matrix logarithm arises from the spectral resolution of each branch of the logarithm.

Definition 1.1.20. The *$k-$th branch of the logarithm*, $\log_k : \mathbb{C}\backslash\{0\} \to \mathbb{C}$, is defined by $\log_k(\lambda) = \log|\lambda| + (\mathrm{Arg}(\lambda) + 2\pi k)i$, where $\log|\lambda|$ is the natural real logarithm of $|\lambda|$ and $\mathrm{Arg}(\lambda) \in (-\pi, \pi]$ is the principal argument of λ. The *principal logarithm* of λ is the logarithm whose imaginary part coincides with $\mathrm{Arg}(\lambda)$. For ease of reading, the principal logarithm of λ will be denoted by $\log(\lambda)$.

Remark 1.1.21. The domain of the branches of the logarithm just defined includes negative numbers. Therefore we can apply the spectral resolution of $\log_k$ to any non-singular square matrix that diagonalizes. However, the derivative of $\log_k$ is not continuous at negative values, so $\log_k$ might not be defined on the spectrum of a non-diagonalizable matrix with negative eigenvalues.

Definition 1.1.22. Given a matrix $A, L \in M_n(\mathbb{C})$ we say that L is a *primary logarithm of A* if it can be obtained as the spectral resolution of $\log_k$ applied to A, $L = \log_k(A)$ for some $k \in \mathbb{Z}$. The primary logarithm arising from the principal logarithm is called the *principal logarithm of A* and is denoted by $\mathrm{Log}(A)$. One can also define the principal logarithm of A by the Mercator series, which is convergent for non-singular matrices with eigenvalues in the disk with radius 1 centered at 1:

$$\mathrm{Log}(A) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(A - Id)^k}{k}.$$

It is known that *all* logarithms of a Jordan block are primary [Gan59]. However, this is not true for generic matrices. Indeed, according to (1.3), one can use different branches of the logarithm on different Jordan blocks and still obtain a matrix logarithms. These logarithms cannot be obtained via the spectral resolution of a single logarithmic function and hence they are called *non-primary logarithms*.

Example 1.1.23 (Logarithms of Id_n)**.** The branches of the logarithm applied to the identity matrix of size n give all its primary logarithms:

$$\log_k(Id_n) = \mathrm{diag}(2\pi ki, \dots, 2\pi ki).$$

However, since $e^{2\pi k\ i} = 1$ for all $k \in \mathbb{Z}$ we have that $\mathrm{diag}(2\pi k_1 i, \dots, 2\pi k_n i)$ is also a logarithm of Id_n for any $k_1, \dots, k_n \in \mathbb{Z}$. Note that this logarithm is primary if and only if $k_1 = \cdots = k_n$. Moreover we deduce from (1.4) that

$$\exp(P\ \mathrm{diag}(2\pi k_1 i, \dots, 2\pi k_n i)\ P^{-1}) = Id_n \text{ for any } k_1, \dots, k_n \in \mathbb{Z}, \\ P \in GL_n(\mathbb{C}).$$

This suggests a procedure to obtain more logarithms of Id_n, none of which will be a diagonal matrix. For example, let us consider the following matrices

$$P_1 = \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \qquad P_2 = \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}.$$

Then,

$$L_1 = P_1 \mathrm{diag}(2\pi i, -2\pi i)\ P_1^{-1} = \begin{pmatrix} 0 & 2\pi \\ -2\pi & 0 \end{pmatrix}$$

and

$$L_2 = P_2 \mathrm{diag}(2\pi i, -2\pi i)\ P_2^{-1} = \begin{pmatrix} 0 & -2\pi \\ 2\pi & 0 \end{pmatrix}$$

are two different non-primary logarithms of Id_2 with the same eigenvalues.

As shown in the previous example, a matrix A may have different non-primary logarithms with the same Jordan form. The following result enumerates all possible logarithms of any non-singular diagonalizable matrix.

Theorem 1.1.24 ([Gan59, Sec. VIII.8]). *Let $A = P\ \mathrm{diag}(\lambda_1, \dots, \lambda_n)\ P^{-1}$ be a non-singular matrix. Then $L \in M_n(\mathbb{C})$ is a logarithm of A if and only if*

$$L = PC\ \mathrm{diag}\big(\log_{k_1}(\lambda_1), \dots, \log_{k_n}(\lambda_s)\big)\ C^{-1}P^{-1} \tag{1.6}$$

for some $k_1, \dots, k_n \in \mathbb{Z}$ and $C \in \mathrm{Comm}^*(\mathrm{diag}(\lambda_1, \dots, \lambda_n))$.

Proof. We start by checking that $exp(L) = A$. Indeed:

$$\begin{aligned} exp(L) &= PC\exp(\mathrm{diag}(\log_{k_1}(\lambda_1), \dots, \log_{k_n}(\lambda_s)))\ C^{-1}P^{-1} \\ &= PC\mathrm{diag}(\lambda_1, \dots, \lambda_s)C^{-1}P^{-1} \\ &= P\mathrm{diag}(\lambda_1, \dots, \lambda_s)P^{-1} = A. \end{aligned}$$

To prove that any logarithm of A can be written as in (1.6) we first note that any logarithm of A must diagonalize. Indeed, let us assume that L is a non-diagonalizable logarithm of A, i.e. $L = \widetilde{P}\ J\ \widetilde{P}^{-1}$ where J is a non-diagonal Jordan form. Then, according to (1.3), $A = \exp(L)$ can be transformed into a block-diagonal matrix with at least one block of size greater than one. According to Lemma 1.1.10, this block does not diagonalize and hence neither does A, which contradicts the hypothesis of the theorem. Therefore we can write $L = \widetilde{P}\ \mathrm{diag}(x_1, \dots, x_n)\ \widetilde{P}^{-1}$ and $\exp(L) = \widetilde{P}\ \mathrm{diag}(e^{x_1}, \dots, e^{x_n})\ \widetilde{P}^{-1}$. This shows that $\lambda_i = e^{x_i}$ for $i = 1, \dots, s$ and hence $x_i = \log_{k_i}(\lambda_i)$ for some $k_i \in \mathbb{Z}$. Moreover, we deduce that $\widetilde{P}$ diagonalizes A and, according to Lemma 1.1.4, this implies that $C = P^{-1}\widetilde{P}$ commutes with $\mathrm{diag}(\lambda_1, \dots, \lambda_n)$. □

The previous result can be extended to almost every non-singular matrix. The exceptions arise because the branches of the logarithm are not defined on the spectrum of matrices with Jordan blocks of size greater than 1 associated with negative eigenvalues (see Remark 1.1.21).

Theorem 1.1.25 ([Gan59, Sec. VIII.8]). *Let $A = P\ J\ P^{-1}$ be a non-singular matrix with eigenvalues $\lambda_1, \dots, \lambda_s \in \mathbb{C} \setminus \{0\}$ and a Jordan form $J = \mathrm{diag}(J_{m_1}(\lambda_1), \dots, J_{m_s}(\lambda_s))$. Assume that the algebraic and geometric multiplicity coincide for any eigenvalue $\lambda_i \in \mathbb{R}_{<0}$ coincide. Then, L is a* *logarithm of A if and only if there exist $k_1, \dots, k_s \in \mathbb{Z}$ and $C \in \mathrm{Comm}^*(J)$ such that*

$$L = PC\ \mathrm{diag}\big(\log_{k_1}(J_{m_1}(\lambda_1)), \dots, \log_{k_s}(J_{m_s}(\lambda_s))\big)\ C^{-1}P^{-1}.$$

Remark 1.1.26. Depending on the Jordan form of A and the choices for $k_1, \dots, k_s$ it may happen that $\mathrm{Comm}^*(\mathrm{diag}(J_{m_1}(\lambda_1), \dots, J_{m_s}(\lambda_s)))$ is included in $\mathrm{Comm}^*\left(\mathrm{diag}\big(\log_{k_1}(J_{m_1}(\lambda_1)), \dots, \log_{k_s}(J_{m_s}(\lambda_s))\big)\right)$. When this holds, there is a unique logarithms of A with the chosen values for $k_1, \dots, k_s$, which can be written as

$$L = P\ \mathrm{diag}\big(\log_{k_1}(J_{m_1}(\lambda_1)), \dots, \log_{k_s}(J_{m_s}(\lambda_s))\big)\ P^{-1}.$$

Moreover, in this case, both A and L have the same eigenvectors. According to Proposition 1.1.5 this occurs, for example, when all the eigenvalues of A are pairwise different (independently of $k_1, \dots, k_s$) or also when $k_1 = k_2 = \dots = k_s$. From this, we obtain the following result:

Corollary 1.1.27. *Let A be a non-singular matrix. For each $k \in \mathbb{Z}$, the primary logarithm $\log_k(M)$ is the unique logarithm of A whose eigenvalues are $k-$th branches of the logarithm of the eigenvalues of A.*

We conclude this section by noting that Theorem 1.1.25 can actually be used for any non-singular matrix by modifying the domain of the branches of the logarithm function in $\mathbb{C}$.

Remark 1.1.28. The branches of the logarithm are usually defined on $\mathbb{C} \setminus (\mathbb{R}_{\leq 0})$ so that they are continuous (actually holomorphic). For any non-singular matrix A there is a ray in the complex plane that does not go through any of its eigenvalues. Hence, we could take another branch cut to define log such that it is continuous on $\sigma(A)$ and then define the k-th branch of the logarithm accordingly. By doing this, the spectral resolution of $\log_k$ would be well-defined in A even if it had negative eigenvalues with different algebraic and geometric multiplicity. In particular, we can define the principal logarithm of any non-singular matrix with negative eigenvalues according to this setting. Moreover, by this procedure, Theorem 1.1.25 can be applied to any non-singular matrix, including those with Jordan blocks with negative eigenvalues of any size.

1.2 MARKOV PROCESSES, MARKOV MATRICES AND RATE MATRICES

The goal of this section is to introduce Markov processes, Markov matrices and rate matrices in order to motivate the embedding problem from the point of view of stochastic processes. Throughout this work we will restrict to Markov chains with a finite state space. The contents in this section can be found in most books on probability applications or random processes such as [GS01], [Asm03] or [Fel08].

1.2.1 Markov chains

We start by introducing Markov chains with the purpose of understanding the nature of Markov matrices, which are needed to define the embedding problem. We consider discrete random variables with a common finite state space $\Sigma = \{y_1, \dots, y_n\}$.

Definition 1.2.1. Let $\mathcal{X} = \{X_t : t \in \mathbb{R}_{\geq 0}\}$ be a family of discrete random variables defined on a common probability space with finite state space Σ and probability measure $\mathbb{P}$. $\mathcal{X}$ is a *continuous-time Markov chain* if

$$\mathbb{P}(X_t = y | X_u : 0 \leq u \leq s) = \mathbb{P}(X_t = x | X_s), \quad \text{for any} \quad s \in [0, t). \tag{1.7}$$

for any index $t \in \mathbb{R}_{>0}$ and any state $y \in \Sigma$.

In this definition, the index variable t is regarded as a continuous variable representing time. Thus, Markov chains are stochastic processes for which future is independent of past, given the present. This conditional independence is known as *memorylessness* and is guaranteed by the *Markov property* given by (1.7).

Given a Markov chain $\mathcal{X}$, the *transition probability* from state $y_i \in \Sigma$ at time t to state $y_j \in \Sigma$ at time $t + s$ is defined as $\mathbb{P}(X_{t+s} = y_j | X_t = y_i)$. Throughout this section we assume that $\mathbb{P}(X_t = y_i) > 0$, for any $t \in \mathbb{R}_{\geq 0}$ and any $y_i \in \Sigma$ so that the conditional probabilities are well defined. Since we assumed that the state space $\Sigma = \{y_1, \dots, y_n\}$ is finite, we can represent the transition probabilities from time t to time $t+s$ by a square matrix of order n:

$$\begin{pmatrix} \mathbb{P}(X_{t+s} = y_1 | X_t = y_1) & \dots & \mathbb{P}(X_{t+s} = y_n | X_t = y_1) \\ \vdots & \ddots & \vdots \\ \mathbb{P}(X_{t+s} = y_1 | X_t = y_n) & \dots & \mathbb{P}(X_{t+s} = y_n | X_t = y_n) \end{pmatrix}.$$

This matrix is called the *transition matrix* from time t to time $t+s$ and we denote it by $M(t, t+s)$.

As transition probabilities can be thought of as the substitution probabilities between states after a given period of time, transition matrices give the probabilities of all possible changes of state occurring after a time interval but give no information about the intermediate states along it.

Next, we show that the product of the transition matrices corresponding to consecutive time intervals lead to the transition probabilities corresponding to the concatenation of these intervals.

Lemma 1.2.2. *For any $t_1, t_2, t_3 \in \mathbb{R}_{\geq 0}$ such that $t_1 < t_2 < t_3$ we have*

$$M(t_1, t_2) M(t_2, t_3) = M(t_1, t_3).$$

Proof. Assuming that the conditional probabilities are well defined and according to their properties, for any states $y_i, y_j \in \Sigma$, we have that

$$\begin{aligned} \mathbb{P}(X_{t_3} = y_j \mid X_{t_1} = y_i) &= \frac{\mathbb{P}(X_{t_3} = y_j,\ X_{t_1} = y_i)}{\mathbb{P}(X_{t_1} = y_i)} \\ &= \sum_{y_k \in \Sigma} \frac{\mathbb{P}(X_{t_3} = y_j,\ X_{t_2} = y_k,\ X_{t_1} = y_i)}{\mathbb{P}(X_{t_1} = y_i)} \\ &= \sum_{y_k \in \Sigma} \frac{\mathbb{P}(X_{t_3} = y_j \mid X_{t_2} = y_k,\ X_{t_1} = y_i)\mathbb{P}(X_{t_2} = y_k,\ X_{t_1} = y_i)}{\mathbb{P}(X_{t_1} = y_i)} \\ &= \sum_{y_k \in \Sigma} \mathbb{P}(X_{t_3} = y_j \mid X_{t_2} = y_k,\ X_{t_1} = y_i)\mathbb{P}(X_{t_2} = y_k \mid X_{t_1} = y_i). \end{aligned}$$

Moreover, $\mathbb{P}(X_{t_3} = y_j \mid X_{t_2} = y_k,\ X_{t_1} = y_i) = \mathbb{P}(X_{t_3} = y_j \mid X_{t_2} = y_k)$ by the Markov property (1.7), which concludes the proof. ☐

1.2.2 Properties of Markov matrices

The entries of the transition matrices are conditional probabilities, and so they lie in the interval $[0, 1]$. Moreover, the rows of a transition matrix sum to one because the sum of all conditional probabilities with the same initial state is equal to 1. Matrices satisfying this property are called Markov matrices.

Definition 1.2.3. A real square matrix M is a *Markov matrix* if its entries are non-negative and all its rows sum to 1. Depending on the context, a Markov matrix might also be referred to as a *transition matrix*, (row-)*stochastic matrix* or *probability matrix*.

Remark 1.2.4. Note that Lemma 1.2.2 yields that the space of $n \times n$ Markov matrices is closed under matrix multiplication and hence it is a multiplicative semi-group.

The Perron-Frobenius theorem [Per07, Fro12] can be used to bound the eigenvalues of positive matrices and of certain classes of non-negative matrices. Next we recall a pair of consequences of this theorem in the setting of Markov matrices.

Proposition 1.2.5. *Let M be a Markov matrix and let $\sigma(M)$ denote the spectrum of M. Then:*

i) $|\lambda| \leq 1$ *for any* $\lambda \in \sigma(M)$.

ii) The vector $\mathbf{1} = (1, \ldots, 1)^t$ *is an eigenvector of M with eigenvalue* 1.

Proof. Let $v = (v_1, \ldots, v_n)^t$ be an eigenvector of M with eigenvalue λ. Take $k \in \{1, \ldots, n\}$ such that $|v_k| = \max_j |v_j|$. Then, we have

$$|\lambda v_k| = \Big|\sum_{j=1}^{n} a_{kj} v_j\Big| \leq \sum_{j=1}^{n} |a_{kj}||v_j| \leq \sum_{j=1}^{n} |a_{kj}||v_k| = \Big(\sum_{i=1}^{n} |a_{ki}|\Big)|v_k| = |v_k|.$$

This proves i). Statement ii) is proven by straightforward computation. □

Remark 1.2.6. According to Perron-Frobenius theorem [Per07], the eigenvalue 1 of any *positive* Markov matrix has multiplicity 1. In this case, its left-eigenvectors are either positive or negative (the same is true for eigenvectors). Moreover, if M is non-negative instead of positive, it is known that the eigenvalue 1 has the same algebraic and geometric multiplicity (see [Mey00, §8.4]).

Definition 1.2.7. A probability distribution $\Pi = (\pi_1, \ldots, \pi_n)$ on the state space Σ is a *stationary distribution* for M if $\Pi M = \Pi$. In particular, a stationary distribution is a left-eigenvector of M with eigenvalue 1. It follows from the previous remark that if M is positive such a distribution exists and is unique. Therefore, in this case, the long term probability of being at state y_k is π_k independently of the initial state.

1.2.3 Homogeneous Markov chains

If we assume that the transition probabilities of a Markov chain $\mathcal{X}$ only depend on the length of the time interval, then it is possible to generate all the transition matrices of $\mathcal{X}$ from a single matrix. A Markov process satisfying this property is said to be homogeneous.

Definition 1.2.8. We say that a continuous-time Markov chain is *(time-) homogeneous* if, for any time values s, t and for any states $y_i, y_j \in \Sigma$, we have $\mathbb{P}(X_{s+t} = y_j \mid X_s = y_i) = \mathbb{P}(X_t = y_j \mid X_0 = y_i)$. In this case, we have $M(0, s) = M(t, t + s)$ for any values of the time variables s and t and we can define $M(t) := M(0, t)$.

Remark 1.2.9. In the case of homogeneous Markov chains, the concatenation of transition matrices given in Lemma 1.2.2 becomes the following identity known as the *Chapman-Kolmogorov equation*:

$$M(t + s) = M(t)M(s). \tag{1.8}$$

Given a homogeneous continuous-time Markov chain $\mathcal{X}$ with state space $\Sigma = \{y_1, \ldots, y_n\}$ we denote by q_{ij} the *instantaneous rate of substitution* from state y_i to y_j. We organize these values on an $n \times n$ matrix Q, where we set $q_{ii} = -\sum_{j \neq i} q_{ij}$. This matrix is called the *instantaneous rate matrix* of $\mathcal{X}$ and is a rate matrix according to the following definition:

Definition 1.2.10. A real square matrix Q is a *rate matrix* if its off-diagonal entries are non-negative and its rows sum to 0.

Remark 1.2.11. Analogously to the case of Markov matrices, we have that $\mathbf{1}$ is an eigenvector with eigenvalue 0 for any rate matrix, because its rows sum to 0.

Next we show that all transition matrices of a homogeneous continuous-time Markov chain arise from its instantaneous rate matrix Q. Moreover, it also claims that Q is unique. For this reason, Q is called the *Markov generator* of the chain.

Theorem 1.2.12. *Let $\mathcal{X} = \{X_t : t \in \mathbb{R}_{\geq 0}\}$ be a homogeneous continuous-time Markov chain with instantaneous rate matrix Q. Then the following are equivalent:*

i) $M(t)$ is the transition matrix from time s to time $s+t$.

ii) $M(t)$ is the unique solution to $M'(t) = M(t)Q$ with $M(0) = Id$.

iii) $M(t) = exp(Qt)$ for all $t \in \mathbb{R}_{\geq 0}$.

Moreover, a matrix $Q \in M_n(\mathbb{R})$ is a rate matrix if and only if $\exp(Qt)$ is a Markov matrix for all $t \in \mathbb{R}_{\geq 0}$.

Proof. Picard-Lindelöf theorem guarantees that the initial value problem arising from a linear system of differential equations has a unique solution. Since, $M(t) = exp(Qt)$ satisfies the differential equation $M'(t) = M(t)\,Q$ with initial condition $M(0) = Id$ then ii) and iii) are equivalent. Hence, it is enough to prove the equivalence between i) and ii) to conclude the proof. For ease of reading, let us denote $\mathbb{P}(X_t = y_j \mid X_0 = y_i)$ by $p_{ij}(t)$. According to the Chapman-Kolmogorov equation (1.8) and using that the rows of Markov matrices sum to one, we can express the transition probabilities at time $t+s$ between any states i and j as:

$$p_{ij}(s+t) = \sum_{k=1}^{n} p_{ik}(s)p_{k,j}(t) = \Big(1 - \sum_{k \neq i} p_{ik}(s)\Big)p_{ij}(t) + \sum_{k \neq i} p_{ik}(s)\; p_{kj}(t).$$

Using that $p_{k,l}(s) \sim s\; q_{kl}$ when s is close to 0 on the expression above we get:

$$\begin{aligned}
p_{ij}(s+t) &\sim \Big(1 - \sum_{k\neq i} s\ q_{i,k}\Big) p_{i,j}(t) + \sum_{k\neq i} s\ q_{i,k}\ p_{k,j}(t) \\
&= p_{i,j}(t) + s\ \Big(\sum_{k\neq i} -q_{i,k}\Big) p_{i,j}(t) + \sum_{k\neq i} s\ q_{i,k}\ p_{k,j}(t) \\
&= p_{i,j}(t) + s\ q_{i,i}\ p_{i,j}(t) + \sum_{k\neq i} s\ q_{i,k} p_{k,j}(t).
\end{aligned}$$

This implies that $M(t+s) \sim M(t) + s\ QM(t)$ when s tends to 0. Taking the limit when s tends to 0 and using the definition of derivative we obtain $M'(t) = QM(t)$. Note that according to the definition of transition matrices we have $M(0) = Id$, which concludes the first part of the proof.
We already proved that if Q is a rate matrix then $M(t) = \exp(Qt)$ is Markov matrix for all $t \geq 0$. To prove the converse, assume that $Q \in M_n(\mathbb{R})$ satisfies that $M(t) = \exp(Qt)$ is a Markov matrix for all $t \in \mathbb{R}_{>0}$. Let us define

$$A(t) = \tfrac{M(t)-Id}{t} \qquad \text{and} \qquad B(t) = \tfrac{M(t)-Id-Q}{t} = \textstyle\sum_{k=2}^{\infty} \tfrac{Qt^k}{k!t}.$$

We have that $Qt = A(t) - B(t)$ for all $t > 0$ because the exponential power series (1.2) is absolutely convergent. Moreover, $A(t)$ is a rate matrix for all $t > 0$ and $\lim_{t\to 0} B(t) = 0$. Therefore Q is a rate matrix. □

Remark 1.2.13. Note that if Q is a rate matrix then Qt is a rate matrix if and only if $t \geq 0$. Thus, the set of $n \times n$ rate matrices is a cone within $M_n(\mathbb{R})$.

1.3 THE EMBEDDING PROBLEM

In this section we introduce the embedding problem posed by Elfving [Elf37] and review some known conditions regarding the existence and uniqueness of solutions to this problem. We also review explicit characterizations of embeddable 2×2 and 3×3 Markov matrices, which were already known before our work.

1.3.1 The embedding problem and the rate identifiability problem

The goal of the embedding problem is to determine if a given Markov matrix M has a homogeneous continuous-time realisation, i.e. to decide whether $M = exp(Qt)$ for some rate matrix Q and some value of time $t \in \mathbb{R}_{\geq 0}$. In Remark 1.2.13 we saw that, if Q is a rate matrix, so is Qt. This motivates the following formulation of the embedding problem.

Definition 1.3.1. A Markov matrix M is *embeddable* if there is a rate matrix Q such that $M = exp(Q)$. In this case, we say that Q is a *Markov generator* for M. The *embedding problem* [Elf37] consists on deciding whether a given Markov matrix is embeddable or not.

Remark 1.3.2. If Q is a Markov generator for M, its eigenvalues are the logarithms of the eigenvalues of M (see Theorems 1.1.24 and 1.1.25).

Example 1.3.3. Consider the following matrices:

$$M = \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{pmatrix} \qquad P = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad N = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Note that both M and N are Markov matrices. Moreover, M diagonalizes with eigendecomposition $M = P\ \mathrm{diag}(1, 0.5)\ P^{-1}$. If we apply the spectral resolution of the principal logarithm to M we obtain:

$$\mathrm{Log}(M) = P\ \mathrm{diag}(\log(1), \log(0.5))\ P^{-1} = \begin{pmatrix} \log(0.5)/2 & -\log(0.5)/2 \\ -\log(0.5)/2 & \log(0.5)/2 \end{pmatrix}.$$

Therefore, M is embeddable because it has a logarithm (the principal logarithm) which is a rate matrix. On the other hand, N diagonalizes with eigendecomposition $N = P\ \mathrm{diag}(1, -1)\ P^{-1}$. It follows from Theorem 1.1.24 that any logarithm of N has a non-real eigenvalue because $\log_k(-1)$ is not real for any $k \in \mathbb{Z}$. Therefore, no logarithm of N is real (and therefore neither a rate matrix) which proves that N is not embeddable.

There are several examples in the literature showing embeddable matrices that admit more than one Markov generator (see for example [Spe67], [Cut73], [SS76], [IRW01], [Dav10]). While the embedding problem is concerned with the existence of Markov generators, the rate identifiability problem focuses on their uniqueness.

Definition 1.3.4. Given an embeddable Markov matrix M, the *rate identifiability problem* consists on deciding whether it has a unique Markov generator. If this is the case, M has *identifiable rates.*

Example 1.3.5. Consider the following matrices:

$$M = \begin{pmatrix} 1-2e^{-6\pi} & 1+e^{-6\pi} & 1+e^{-6\pi} \\ 1+e^{-6\pi} & 1-2e^{-6\pi} & 1+e^{-6\pi} \\ 1+e^{-6\pi} & 1+e^{-6\pi} & 1-2e^{-6\pi} \end{pmatrix}, \qquad P = \begin{pmatrix} 1 & -1-i & 1+i \\ 1 & i & -i \\ 1 & 1 & 1 \end{pmatrix}.$$

A straightforward computation shows that $M = P\ \mathrm{diag}(1,\lambda,\lambda)\ P^{-1}$, with $\lambda = -e^{-6\pi}$. Moreover, both $Q_1 = P\ \mathrm{diag}(0, \log(\lambda), \log_{-1}(\lambda))P^{-1}$ and $Q_2 = P\ \mathrm{diag}(0, \log_{-1}(\lambda), \log(\lambda))P^{-1}$ are non-primary logarithms of M and are rate matrices. Indeed:

$$Q_1 = \begin{pmatrix} -4\pi & \pi & 3\pi \\ 7\pi/3 & -11\pi/3 & 4\pi/3 \\ 5\pi/3 & 8\pi/3 & -13\pi/3 \end{pmatrix}, \qquad Q_2 = \begin{pmatrix} -4\pi & 3\pi & \pi \\ 5\pi/3 & -13\pi/3 & 8/3\pi \\ 7\pi/3 & 4\pi/3 & -11\pi/3 \end{pmatrix}.$$

Hence, M is an embeddable Markov matrix whose rates are not identifiable.

1.3.2 Known conditions on the existence and uniqueness of Markov generators

Here, we review the study on real logarithms of real matrices developed in [Cul66]. Since both Markov matrices and rate matrices have real entries, we specialize these results in our setting of real logarithms of Markov matrices. Several known necessary conditions for the existence of Markov generators arise from this work. We also state some known results regarding rate identifiability that shall be used later on.

Proposition 1.3.6 ([Cul66])**.** *Let M be a real square matrix.*

i) If there exists a real logarithm of M, then $\det(M) > 0$ and each Jordan block of M associated with a negative eigenvalue occurs an even number of times.

ii) If all the eigenvalues of M are positive and no Jordan block appears more than once in its Jordan canonical form, then the principal logarithm of M is its unique real logarithm.

Proof. We first note that for any given $\lambda \in \mathbb{C} \setminus \{0\}$ and $k \in \mathbb{Z}$, we have

$$\overline{\log_k(\lambda)} = \begin{cases} \log_{-k}(\overline{\lambda}) & \text{if } \lambda \in \mathbb{C} \setminus \mathbb{R}_{<0}, \\ \log_{-k-1}(\lambda) & \text{if } \lambda \in \mathbb{R}_{<0}. \end{cases} \tag{1.9}$$

i) Assume that M has a Jordan block with a negative eigenvalue λ that occurs an odd number of times and let L be a logarithm of M. By changing the branch cut of the logarithm (see Remark 1.1.28), Lemma 1.1.10 can be applied to every $k-$th branch of the logarithm $f = \log_k$ in any Jordan block $J_n(\lambda)$, $n \geq 1$. Since $\lambda < 0$, we deduce from Theorem 1.1.25 that the Jordan form of L has an odd number of Jordan blocks whose eigenvalues are a non-real logarithm of λ. Together with (1.9) this implies that L is not a real matrix.

ii) For positive numbers, the principal logarithm is the only branch of the logarithm that produces a real logarithm. The claim follows immediately from Theorem 1.1.25 and Proposition 1.1.27. □

Remark 1.3.7. The converse of both statements in this proposition are also true (see Theorems 1 and 2 in [Cul66]).

As a consequence, one obtains the following characterization for the embeddability of Markov matrices with pairwise different real eigenvalues.

Corollary 1.3.8 ([SS76])**.** *Let M be a Markov matrix with* real pairwise different *eigenvalues. Then, M is embeddable if and only if* $\text{Log}(M)$ *is a rate matrix. In this case, M has identifiable rates and all its eigenvalues are positive.*

Proof. Under the assumption and according to Proposition 1.3.6 i), if M has a negative eigenvalue then it has no real logarithms. If M has pairwise different positive eigenvalues then the only real logarithm of M is its principal logarithm by Proposition 1.3.6 ii) and hence, no other logarithm of M can be a rate matrix. □

This shows that the results by Culver [Cul66] on real logarithms have an impact not only in the embedding problem but also on the identifiability of rates. Indeed, if M has different real eigenvalues then the previous corollary guarantees that there is *at most one* Markov generator. Together with this, the next result quantifies the set of real logarithms for real matrices in general.

Corollary 1.3.9 ([Cul66]). *Let M be a real square matrix and assume that the equation $M = \exp(Q)$ has more than one solution. Then, there are an infinite number of real solutions Q, which are:*

i) Countable, if the Jordan canonical form of M has no repeated Jordan block. In this case, M necessarily has a non-real eigenvalue.

ii) Uncountable, if the Jordan canonical form of M contains at least two Jordan blocks of the same size with the same eigenvalue.

Together with Proposition 1.3.6, the result above suggests that there might be Markov matrices with infinitely many real logarithms (which can be a rate matrix or not). However, there are some other known conditions, besides those of Corollary 1.3.8, that guarantee the uniqueness of a Markov generator.

Theorem 1.3.10 ([Cut72, Cut73]). *Let M be Markov matrix satisfying any of the following conditions:*

i) $\min_i\{m_{i,i}\} > 0.5$, *or*

ii) $\det(M) > e^{-\pi}$.

Then, M is embeddable if and only if its principal logarithm is a rate matrix. In this case, M has identifiable rates.

Remark 1.3.11. There are other known sufficient conditions that guarantee that the only possible Markov generator of a Markov matrix is its principal logarithm. For example, this is satisfied if M satisfies $\det(M) > 0.5$ and $\|M - Id\| < 0.5$ for some multiplicative norm [IRW01].

The previous theorem illustrates that the embeddability of any Markov matrix close enough to the identity is determined by its principal logarithm. Moreover, if such a matrix is embeddable it has identifiable rates. In the following example, we use this to show that for $n \geq 3$ there are matrices close to the identity matrix that are not embeddable.

Example 1.3.12. Let $M = \operatorname{diag}(Id_{n-3}, A)$ where

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\varepsilon_1 & \varepsilon_1 \\ \varepsilon_2 & 0 & 1-\varepsilon_2 \end{pmatrix} \text{ with } \varepsilon_1, \varepsilon_2 \in (0,1) \text{ satisfying } \varepsilon_1 \neq \varepsilon_2.$$

Then, $\operatorname{Log}(M) = \operatorname{diag}(0, \operatorname{Log}(A))$ where 0 denotes the zero matrix of size $n-3$ and $\operatorname{Log}(A)$ is the principal logarithm of A,

$$\operatorname{Log}(A) = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\varepsilon_2 \log(1-\varepsilon_1) - \varepsilon_1 \log(1-\varepsilon_2)}{-(\varepsilon_2-\varepsilon_1)} & \log(1-\varepsilon_1) & \frac{\varepsilon_1 \log(1-\varepsilon_2) - \varepsilon_1 \log(1-\varepsilon_1)}{-(\varepsilon_2-\varepsilon_1)} \\ -\log(1-\varepsilon_2) & 0 & \log(1-\varepsilon_2) \end{pmatrix}.$$

Note that if $\varepsilon_2 > \varepsilon_1$ the numerator of the entry $\operatorname{Log}(A)_{2,1}$ is positive and its denominator is negative. On the contrary, if $\varepsilon_1 > \varepsilon_2$ the numerator is negative and the denominator is positive. Hence, $\operatorname{Log}(M)$ is not a Markov generator because $\operatorname{Log}(A)_{2,1} < 0$. Therefore, by taking $\varepsilon_1 \neq \varepsilon_2$ close enough to zero we have that M is a non-embedabble matrix as close to Id_n as wanted.

1.3.3 Embeddability of 2×2 and 3×3 Markov matrices

In this section we deal with the case of 2×2 and 3×3 Markov matrices, for which characterizations of embeddability are already known.

Case $n = 2$

Since 1 is an eigenvalue of any Markov matrix, it turns out that 2×2 Markov matrices only have real eigenvalues. Hence, Corollary 1.3.8 and Theorem 1.3.10 can be used to solve the embedding problem for any 2×2 Markov matrix. Moreover, these results also show that any embeddable 2×2 Markov matrix has identifiable rates.

On the other hand, the embeddability of 2×2 Markov matrices was already characterized by [Kin62] some years before the results presented above.

Moreover, his solution is simpler as it does not require the computation of $\mathrm{Log}(M)$.

Theorem 1.3.13 ([Kin62]). *Let M be a 2×2 Markov matrix. Then the following are equivalent:*

i) *M is embeddable.*

ii) $\det(M) > 0$.

iii) $\mathrm{tr}(M) > 1$.

Proof. By Proposition 1.2.5 we have that either $M = Id_2$ or M diagonalizes with two different real eigenvalues, 1 and $\lambda \in [-1, 1)$. If $M = Id_2$ then the statement holds owing to the fact that $\mathrm{Log}(Id_2)$ is the 2×2 zero matrix (see Example 1.1.23). Assume now that $\lambda \neq 1$. In this case, there is $P \in GL_2(\mathbb{R})$ such that $M = P\ \mathrm{diag}(1, \lambda)\ P^{-1}$. Since both the trace and the determinant are endomorphism invariants we have $\det(M) = \lambda$, $\mathrm{tr}(M) = 1+\lambda$ and hence we get the equivalence between statements ii) and iii). If M has a Markov generator then it has a real logarithm. In this case, we infer from Remark 1.1.18 and Proposition 1.3.6 i) that $\lambda > 0$, thus i) implies ii). Finally, let us assume that $\det(M) = \lambda > 0$ and compute the principal logarithm of M:

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

Note that $M - Id$ is a rate matrix. Moreover, since $\lambda \in (0, 1)$ we have that $\log(\lambda)/(\lambda - 1) > 0$ and hence we infer from Remark 1.2.13 that $\mathrm{Log}(M)$ is a rate matrix □

Case $n = 3$

The solution to the embedding problem for 3×3 Markov matrices can be split into different cases according to the Jordan canonical form of the Markov matrix. Corollary 1.3.8 gives sufficient and necessary conditions to guarantee the embeddability of 3×3 Markov matrices with different real eigenvalues. The following result deals with the case of Markov matrices with a conjugated pair of complex eigenvalues or a repeated positive eigenvalues. The case of repeated negative eigenvalues shall be treated afterwards.

Theorem 1.3.14 ([Cut73]). *Let $M = P \operatorname{diag}(1, \mu, \overline{\mu})\ P^{-1}$ be a Markov matrix. Then*

i) If $\mu \in \mathbb{R}_{>0}$, M is embeddable if and only if $\operatorname{Log}(M)$ is a rate matrix.

ii) If $\mu \in \mathbb{C} \setminus \mathbb{R}$, M is embeddable if and only if $\operatorname{Log}(M)$ is a rate matrix or $P \operatorname{diag}(0, \log_{-1}(\mu), \log_{-1}(\overline{\mu}))\ P^{-1}$ is a rate matrix.

iii) If $\mu \in \mathbb{R}_{<0}$ and M is embeddable then $P \operatorname{diag}(0, \log|\mu|, \log|\mu|)\ P^{-1}$ is a rate matrix.

In [Car95] it is shown that the embeddability of 3×3 Markov matrices with a repeated negative eigenvalue is equivalent to the existence of a square root of the Markov matrix satisfying several constraints. In spite of that, finding such a square root and finding Markov generators turn out to be problems with a similar difficulty for a matrix with a repeated eigenvalue, because there is an uncountable amount of non-primary logarithms and non-primary roots.

The embeddability of 3×3 Markov matrices with a repeated negative eigenvalue was explicitly characterized for the first time in [CC11]. The solution provided there shows that the embedding problem can become quite complex in the case of repeated eigenvalues:

Theorem 1.3.15 ([CC11, Theorem 2.6]). *Let $M = P\operatorname{diag}(1, \lambda, \lambda)P^{-1}$ be a Markov matrix with $\lambda \in [-1, 0)$. Let $(v_1, v_2, v_3) \in \mathbb{R}^3$ be the left eigenvalue of M with eigenvalue 1 satisfying $v_1 + v_2 + v_3 = 1$ and denote by w the minimum of v_1, v_2, v_3.*

i) If $\frac{1}{v_1}, \frac{1}{v_2}, \frac{1}{v_3}$ are realizable as the sides of a triangle then

$$M \text{ is embeddable if and only if } \sqrt{\frac{4v_1v_2v_3}{(v_1v_2+v_1v_3+v_2v_3)^2} - 1} \geq \frac{\pi}{-\log|\lambda|}.$$

ii) If $\frac{1}{v_1}, \frac{1}{v_2}, \frac{1}{v_3}$ *are not realizable as the sides of a triangle, then*

$$M \text{ is embeddable if and only if } \sqrt{\tfrac{w}{1-w}} \geq \tfrac{\pi}{-\log|\lambda|} .$$

Remark 1.3.16. Corollary 2.3 in [CC11] shows that $v_1, v_2, v_3 > 0$, so $w > 0$.

From Proposition 1.2.5 we have that any non-diagonalizable 3×3 Markov matrix M has Jordan form $\mathrm{diag}(1, J_2(\lambda))$ with $\lambda \neq 1$. Moreover, according to Proposition 1.3.6, such a matrix is embeddable if and only if $\mathrm{Log}(M)$ is a rate matrix. This, together with Corollary 1.3.8, Theorem 1.3.14 and Theorem1.3.15, solves completely the embedding problem for 3×3 Markov matrices.

To conclude this section we want to point out that, in [Joh74, Cor. 1.2], the author rewrites the necessary and sufficient conditions for the embeddability of 3×3 Markov matrices given by Corollary 1.3.8 and Theorem 1.3.14 ii) in terms of the entries of the Markov matrix and its eiganvalues. Analogously, [Joh74, Prop. 1.4] gives another characterization of 3×3 embeddable matrices with a repeated real eigenvalue (diagonalizable or not) equivalent to that in 1.3.14 i, which consists on checking whether the principal logarithm of the Markov matrix is a rate matrix or not.

1.4 MATHEMATICAL MODELS FOR NUCLEOTIDE SUBSTITUTION

In this section we explain how Markov processes can be used to model the evolution of DNA sequences. This can be found in any book related to algebraic statistics in the context of nucleotide substitution models such as [AR04], [PS05], [Ste16] or [Sul18].

The *deoxyribonucleic acid (DNA)* is a molecule found in the nucleus of the cells of living organisms. The DNA carries all the genetic information of the organism, which contains the instructions for its development, functioning, growth and reproduction. The DNA has a double helix structure, composed by two strands of smaller units, called *nucleotides*. There are four different nucleotides which can be found in the DNA strands, *adenine* ($\mathtt{A}$), *guanine* ($\mathtt{C}$), *cytosine* ($\mathtt{C}$) and *thymine* ($\mathtt{T}$). Therefore, it is usual to represent DNA strands as a sequence of characters in the alphabet $\{\mathtt{A},\mathtt{G},\mathtt{C},\mathtt{T}\}$. Both DNA strands are linked via hydrogen bonds between their nucleotides according to the pairings $\mathtt{A}-\mathtt{T}$ and $\mathtt{C}-\mathtt{G}$ (*Watson-Crick base pairing*). Hence, there is a complementarity relationship between the strands.

During the replication of the DNA, some changes in the sequence may occur. For example, a nucleotide might be substituted by another one (this is known as single nucleotide polymorfism). Nucleotide substitution models are simplified models for the evolution of DNA sequences. In these models, one usually assumes that the substitution of nucleotides occurs randomly and following a Markov process.

1.4.1 Nucleotide substitution models

We can model the substitution of nucleotides in an evolutionary process by the conditional probabilities that a nucleotide is substituted by another one. The random variables at the beginning and at the end of this process, denoted by X and Y respectively, take values in the set of nucleotides. If we fix the order $\mathtt{A},\mathtt{G},\mathtt{C},\mathtt{T}$ in the states, the corresponding transition matrix is defined as

$$M = \begin{pmatrix} \mathbb{P}(Y=\mathtt{A}|X=\mathtt{A}) & \mathbb{P}(Y=\mathtt{G}|X=\mathtt{A}) & \mathbb{P}(Y=\mathtt{C}|X=\mathtt{A}) & \mathbb{P}(Y=\mathtt{T}|X=\mathtt{A}) \\ \mathbb{P}(Y=\mathtt{A}|X=\mathtt{G}) & \mathbb{P}(Y=\mathtt{G}|X=\mathtt{G}) & \mathbb{P}(Y=\mathtt{C}|X=\mathtt{G}) & \mathbb{P}(Y=\mathtt{T}|X=\mathtt{G}) \\ \mathbb{P}(Y=\mathtt{A}|X=\mathtt{C}) & \mathbb{P}(Y=\mathtt{G}|X=\mathtt{C}) & \mathbb{P}(Y=\mathtt{C}|X=\mathtt{C}) & \mathbb{P}(Y=\mathtt{T}|X=\mathtt{C}) \\ \mathbb{P}(Y=\mathtt{A}|X=\mathtt{T}) & \mathbb{P}(Y=\mathtt{G}|X=\mathtt{T}) & \mathbb{P}(Y=\mathtt{C}|X=\mathtt{T}) & \mathbb{P}(Y=\mathtt{T}|X=\mathtt{T}) \end{pmatrix}.$$

A *nucleotide substitution model* is specified by a subset of the set of 4×4 Markov matrices. These models do not take time into consideration. When we consider homogeneous continuous-time models we will state it explicitly (see Section 1.4.2).

Most nucleotide substitution models are simplifications of this general model and assume identities between the transition parameters, usually motivated by biochemical properties of the DNA or simply by mathematical or computational convenience. Next, we briefly list some of these models, starting from the most simple and increasing the complexity until considering the General Markov model.

The Jukes-Cantor model

The simplest nucleotide substitution model is the Jukes-Cantor model, which considers that all substitutions have the same probability to occur and only distinguishes between silent (the nucleotide remains the same at the end of the process) and non-silent substitutions [JC69].

Definition 1.4.1. We say that a 4×4 real matrix is a *Jukes-Cantor matrix* (*JC* matrix for short) if all its off-diagonal entries are equal:

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

The *Jukes-Cantor model* (*JC model* for short) is the nucleotide substitution model whose transition matrices are JC Markov matrices.

The Kimura models

Depending on their chemical composition, nucleotides can be classified into purines (`A` and `G`) and pyrimidines (`C` and `T`). According to this, substitutions are categorized as *transitions* (a substitution between purines or between pyrimidines) or *transversions* (a substitution of a purine by a pyrimidine or vice versa). The Kimura models are nucleotide substitution models that give different substitution probabilities depending on whether they correspond to transitions or transversions. The *Kimura 2-parameter model* [Kim80] assumes that all transitions have the same probability and also that all transversions occur with the same probability. The *Kimura 3-parameter model* [Kim81] further assumes two different substitution probabilities for transitions depending on whether the original nucleotide is substituted by its complementary or not (see Figure 1.1).

Definition 1.4.2. A *Kimura 3-parameter matrix* (*K3P* matrix for short) is a 4×4 real matrix with the following shape:

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

For ease of reading we will use the notation $K(a, b, c, d)$ to denote a matrix with the structure above. If $c = d$ we say that such a matrix is a *Kimura 2-parameter* matrix (*K2P* matrix for short).

The *Kimura 3-parameter model* (*K3P model* for short) is the nucleotide substitution model whose transition matrices are K3P matrices. The *Kimura 2-parameter model* (*K2P model* for short) is defined analogously.

Remark 1.4.3. Note that JC matrices and K2P matrices are particular cases of K3P matrices. Thus the corresponding models are submodels of the K3P model. Moreover, if $M = K(a, b, c, d)$ is a Markov matrix then $a + b + c + d = 1$. Thus, $\mathbf{1}$ is a left-eigenvector with eigenvalue 1 (see Proposition 1.2.5). Therefore, the uniform distribution $\Pi = (1/4, 1/4, 1/4, 1/4)$ is said to be the stationary distribution of the K3P model and its submodels (as it is the stationary distribution for all positive K3P Markov matrices).

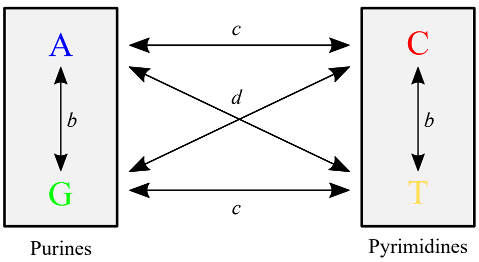

Figure 1.1: Substitution probabilities according to the Kimura 3-parameter model. For the Kimura 2-parameter model we have $c = d$ and for the Jukes-Cantor model, $b = c = d$.

The strand symmetric model

The *strand symmetric model* is a nucleotide substitution model that takes into account the complementary pairs of nucleotides $\texttt{A} - \texttt{T}$, $\texttt{C} - \texttt{G}$ [YP04, CS05] . Due to the molecular structure of the DNA, this implies that, whenever there is a substitution on a nucleotide in one of the strands, there is also a substitution on the corresponding complementary nucleotide in the other strand .

Definition 1.4.4. A strand symmetric matrix (*SS* matrix for short) is a 4×4 real matrix with the following form:

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

The *strand symmetric model* (*SS model* for short) is the nucleotide substitution model whose transition matrices are SS matrices.

The General Markov model

The most general nucleotide substitution model is the *general Markov model*, which assumes that each substitution might have a different probability to occur. Therefore, this model considers different parameters for each possible substitution and admits any Markov matrix as a transition matrix.

1.4.2 Nucleotide substitution models in continuous-time

In the setting of nucleotide substitution models in continuous-time, the constraints of the model are assumed on the instantaneous substitution rates rather than on the transition probabilities. In order to keep the model tractable it is usually assumed that the instantaneous substitution rates are constant throughout time (homogeneity assumption). In this case, evolution is modelled as a homogeneous Markov process in continuous-time.

Definition 1.4.5. The *continuous-time Jukes-Cantor model* is the homogeneous continuous-time model whose rate matrices are JC matrices. Similarly, we consider the *continuous-time Kimura 2-Parameter model*, the *continuous-time Kimura 3-Parameter model*, the *continuous-time strand symmetric model* and the *continuous-time general Markov model*.

Remark 1.4.6. The Jukes-Cantor model and both Kimura models were originally introduced in the setting of continuous-time by describing the structure of the rate matrices (see [JC69, Kim80, Kim81]). Hence, in the context of evolutionary biology, the notation JC69, K2P and K3P usually denotes homogeneous continuous-time models.

Expressing the model constraints in terms of the probabilities of substitution between states or in terms of the instantaneous rates of substitution leads to two different versions of the same model connected by the embedding problem. A related problem is that of deciding when a transition matrix subjected to model constraints admits a Markov generator with the same restrictions on its entries. This problem has been deeply studied recently (see [Mat08, AKK21]).

Definition 1.4.7. Given a homogeneous continuous-time nucleotide substitution model $\mathcal{M}$, we say that a Markov matrix is *model-embeddable* (or $\mathcal{M}$*-embeddable*) if it is embeddable and at least one of its Markov generators belongs to $\mathcal{M}$.

1.4.3 Phylogenetic trees

Phylogenetics is the subfield of evolutionary biology that studies the evolutionary relationships among species using genomic data. Charles Darwin proposed in his celebrated book *On the Origin of Species* [Dar59] that all the living beings in the Earth are descendants of a single species, so-called the *last universal common ancestor*. According to this, it seems natural to represent the living species and its ancestors in a tree-like structure, known as *tree of life*, which represents the evolutionary relationships (*phylogenies*) among species.

Definition 1.4.8. A *tree* is a connected acyclic graph. We say that a tree is *rooted* if all the edges of the graph are directed away from a fixed node, which is called the *root* of the tree. The *leaves* of a tree are its nodes of degree one (by degree of a node we mean the number of edges incident to it). A *phylogenetic tree* is a tree whose leaves are labelled within a given set of living species (or other taxonomies). Each edge (or *branch*) of such a tree represents an ancestor-descendant relationship between the connected nodes, so that the inner nodes correspond to ancestors of the species at the leaves.

The main goal in phylogenetics is to reconstruct the evolutionary history of a given number of living species (or other taxa). This is usually expressed by means of *phylogenetic tree*. In this context, the evolution of DNA sequences can be modelled by a Markov process in a phylogenetic tree and the Markov property states that the evolution at different lineages is independent given their common ancestor. By further assuming that each site in a DNA sequence evolves independently from each other and all follow the same Markov process (independently and identically distributed), one can model the evolution of DNA sequences on a phylogenetic tree by modelling a single position. This is done by assigning a distribution $\Pi = (\pi_{\mathtt{A}}, \pi_{\mathtt{G}}, \pi_{\mathtt{C}}, \pi_{\mathtt{T}})$ at the root of the tree and specifying 4×4 transition matrices $M^{(e)}$ at each edge e of the tree. These are called the *substitution parameters* of this Markov process on the phylogenetic tree.

Remark 1.4.9. The length of a branch in a phylogenetic tree usually represents the expected number of elapsed nucleotide substitutions per site that have occurred along the Markov process on that branch. If the uniform distribution is a stationary distribution for $M^{(e)}$, then the branch length of e can be approximated by $-\frac{\log(\det(M^{(e)}))}{4}$ [BH87].

Example 1.4.10. Let X_1, X_2, X_3 be random variables with a common state space $\{\mathtt{A}, \mathtt{G}, \mathtt{C}, \mathtt{T}\}$ and let $M^{(e_i)} = K(1 - b_i - c_i - d_i, b_i, c_i, d_i)$ be K3P Markov matrices for $i = 1, 2, 3, 4$. Figure 1.2 represents a nucleotide substitution process in a phylogenetic tree following the K3P model:

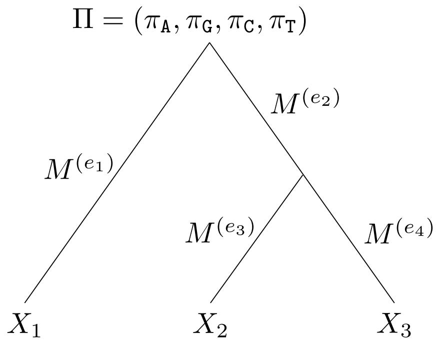

Figure 1.2: Markov process on a phylogenetic tree.

The substitution parameters for this evolutionary process are the distribution Π at the root (which is usually assumed to be uniform so that it coincides with the stationary distribution of the K3P model) and b_i, c_i, d_i for $i = 1, 2, 3, 4$. Using the Markov property on the tree, one can compute the joint distribution of (X_1, X_2, X_3) from the substitution parameters.

It is known that the set of transition matrices of a models needs to be multiplicatively closed in order to be consitent with the concatenation of evolutionary processes(see [SFSJ12], [FSSJW15], [SJFS$^+$12]). Taking this into account, some phylogenetic reconstruction methods aim to recover the substitution parameters from the observed data (see for example [KK19]). Moreover, in the setting of continuous-time models, for each edge e we have $M^{(e)} = \exp(Q_e t_e)$ for some rate matrix Q_e and time $t_e > 0$ and some phylogenetic reconstruction methods aim to recover $Q_e t_e$ (in general it is not possible to recover them independently) instead of $M^{(e)}$. Thus, in this context rate identifiability is crucial.

The reader may note that there are transition matrices, such as permutation matrices, which might have no sense from a biological point of view. Thus, not all Markov matrices within a nucleotide substitution model $\mathcal{M}$ are "biologically meaningful". In general, transition matrices related to the evolution of a DNA sequence should be close to the identity matrix to allow a more robust inference.

To conclude this section, we introduce next several sets of transition matrices that have interest for phylogenetic inference in relation with what we have explained.

Definition 1.4.11. For any nucleotide substitution model $\mathcal{M}$, we define the following sets:

$\Delta^{\mathcal{M}}$ The set of all Markov matrices in the model.

$\Delta^{\mathcal{M}}_{\mathrm{dlc}}$ The set of Markov matrices in the model whose diagonal entries are the largest entries in each column. These matrices are called *diagonal largest in column*, *DLC* for short. Having invertible DLC matrices is a necessary condition for the the identifiability of the substitution parameters in a phylogenetic tree [Cha96].

$\Delta^{\mathcal{M}}_{\mathrm{dd}}$ The set of all $M \in \Delta^{\mathcal{M}}$ such that the probability of not mutating is higher than the probability of mutating, i.e. $M_{ii} \geq 0.5$ for all i. These matrices are said to be *diagonally-dominant* matrices. If embeddable, these matrices have identifiable rates (see the first claim in Theorem 1.3.10).

$\Delta^{\mathcal{M}}_{\mathrm{Id}}$ The set of all $M \in \Delta^{\mathcal{M}}$ in the connected component of the identity matrix when we remove from $\Delta^{\mathcal{M}}$ all matrices with determinant equal to 0. This corresponds to the set of Markov matrices with positive eigenvalues if all the transition matrices in $\Delta^{\mathcal{M}}$ have real eigenvalues. On the contrary, if the model admits transition matrices with non-real eigenvalues, then $\Delta^{\mathcal{M}}_{\mathrm{Id}}$ is the set of Markov matrices with positive determinant. This set necessarily includes the multiplicative closure of the transition matrices in the continuous-time version of the model [SFSJ12].

$\Delta^{\mathcal{M}}_{\mathrm{emb}}$ The set of all embeddable Markov matrices in the model. That is, the set of transition matrices that admit a homogeneous continuous-time realisation.

Since the the model General Markov model does not impose any restrictions on transition matrices, if $\mathcal{M}$ is the General Markov model, we will omit it from the notation for ease of reading.

Remark 1.4.12. Note that if a matrix is diagonally-dominant, then its off diagonal entries are smaller than or equal to 0.5. Hence, $\Delta^{\mathcal{M}}_{\mathrm{dd}} \subseteq \Delta^{\mathcal{M}}_{\mathrm{dlc}} \subseteq \Delta^{\mathcal{M}}$. Also note that, if all the transition matrices in $\Delta^{\mathcal{M}}$ have real eigenvalues then $\Delta^{\mathcal{M}}_{\mathrm{Id}}$ corresponds to the set of Markov matrices with positive eigenvalues. On the contrary, if the model admits transition matrices with non-real eigenvalues, then $\Delta^{\mathcal{M}}_{\mathrm{Id}}$ is the set of Markov matrices with positive determinant.

Remark 1.4.13. Note that every embeddable matrix is the product of embeddable matrices close to the identity matrix. Indeed, if $M = \exp(Q)$ is an embeddable matrix, we have that $Q_n := \frac{1}{n}Q$ is a rate matrix for any $n \geq 1$ (see Remark 1.2.13). Therefore, $M = \exp(Q_n)^n$ appears as the n-th power of a Markov matrix. Moreover, we can take n big enough so that $\exp(Q_n)$ is as close to Id as wanted. This justifies that all embeddable matrices are biologically meaningful, including those with negative eigenvalues or small determinant.

2

EMBEDDABILITY AND RATE IDENTIFIABILITY OF GENERIC MARKOV MATRICES

In this chapter we address the embedding problem for $n \times n$ Markov matrices with pairwise different eigenvalues (not necessarily real) for any $n \in \mathbb{N}$. Note that this is a dense subset within the set of $n \times n$ Markov matrices. Since the case of real eigenvalues is already solved by Corollary 1.3.8 we focus on Markov matrices with non-real eigenvalues.

In the first section we derive some bounds for the eigenvalues of rate matrices. In the second section, we use these bounds to relax the conditions given in Theorem 1.3.10 ii), which guarantee that the principal logarithm is the only possible Markov generator of a given Markov matrix. In the third section, we give a bound on the number of Markov generators in terms of the spectrum of a Markov matrix. Based on this, we establish a criterion for deciding whether a generic Markov matrix (different eigenvalues) is embeddable (Theorem 2.3.3) and, in this case, we propose an algorithm that lists all its Markov generators (Algorithm 2.3.5).

2.1 BOUNDS ON THE EIGENVALUES OF RATE MATRICES

In 1945 Kolmogorov posed the problem of describing the set of all the possible eigenvalues of a Markov matrix [Swi72, p.2]. Note that both the Perron-Frobenius theorem for positive matrices and the Gershgorin circles theorem for general matrices [Ger31] were already stated at that time, so it was known that the solution to this problem was a region in the complex plane included in the unit disc centered at 0 (see the first claim in Proposition 1.2.5). The first description of this region was implicitly given by Karpelevich in [Kar51] (see also [DD45] and [DD46]). In particular, Karpelevich proved that any non-real eigenvalue λ of an $n \times n$ Markov matrix satisfies:

$$\left(\frac{1}{2} + \frac{1}{n}\right)\pi \leq |\operatorname{Arg}(\lambda - 1)|. \tag{2.1}$$

Recall that Lemma 1.1.12 and Theorem 1.2.12 provide a tool to translate results on eigenvalues of Markov matrices into rate matrices. Using this, Runnenburg obtained the following result by adapting (2.1) to rate matrices.

Lemma 2.1.1 ([Run62])**.** *Let $Q \in M_n(\mathbb{R})$ be a rate matrix. Then, for any eigenvalue $\lambda \in \sigma(Q)$ we have*

$$\left(\frac{1}{2} + \frac{1}{n}\right)\pi \leq |\operatorname{Arg}(\lambda)|. \tag{2.2}$$

Remark 2.1.2. In [Run62] it is also shown that the only rate matrices $Q = (q_{ij})$ with at least one eigenvalue $\lambda \neq 0$ for which (2.2) is tight are given (after a suitable reordering of both rows and columns) by:

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

We use Runnenburg's result to provide bounds on the imaginary part of the complex eigenvalues of rate matrices. To this end, for any rate matrix Q of size 3×3 or larger and any eigenvalue $\lambda \in \sigma(Q)$, we define

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

and

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

The following result bound the real and imaginary part of λ and shows that $b_n(\lambda)$ is well-defined (see (2.3)).

Lemma 2.1.3. *Let Q be an $n \times n$ rate matrix. Then for any eigenvalue $\lambda \in \sigma(Q)$ we have*

i) $\mathrm{Re}(\lambda) \leq 0$ *and, if* $\lambda \notin \mathbb{R}$*, then* $\frac{\mathrm{tr}(Q)}{2} \leq \mathrm{Re}(\lambda) \leq 0$.

ii) *If* $\lambda \notin \mathbb{R}$*, then* $n \geq 3$ *and* $|\mathrm{Im}(\lambda)| \leq b_n(\lambda) \leq B_n$.

Proof.

i) If Q is a rate matrix, then $\exp(Q)$ is a Markov matrix by Theorem 1.2.12. In particular, the eigenvalues of Q are logarithms of the eigenvalues of a Markov matrix (see Lemma 1.1.12). Using that $|e^{\lambda}| = e^{\mathrm{Re}(\lambda)}$ together with the fact that the modulus of the eigenvalues of a Markov matrix is bounded by 1 (see Proposition 1.2.5) we deduce that $\mathrm{Re}(\lambda) \leq 0$ for any $\lambda \in \sigma(Q)$. Note that

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

Therefore, $\mathrm{tr}(Q) \leq \mathrm{Re}(\lambda)$. Moreover, if $\lambda \notin \mathbb{R}$, then $\mathrm{Re}(\lambda)$ appears twice in this expression because non-real eigenvalues of Q appear in conjugated pairs. Thus, $\mathrm{Re}(\lambda) \geq \mathrm{tr}(Q)/2$.

ii) We know that 0 is an eigenvalue of Q (see Remark 1.2.11). Moreover, since Q is a real matrix $\overline{\lambda} \in \sigma(Q)$. Hence, Q has at least three different eigenvalues. Now, note that from the inequalities obtained in 2.1.3) it is straightforward that

$$2\,\mathrm{tr}(Q)\,\mathrm{Re}(\lambda) - (\mathrm{Re}(\lambda))^2 \geq 0 \tag{2.3}$$

In particular $b_n(\lambda)$ is well-defined. Next we show that for any non-real eigenvalue $\lambda \in \sigma(Q)$ we have

$$|\,\mathrm{Im}(\lambda)| \leq \sqrt{2\,\mathrm{tr}(Q)\,\mathrm{Re}(\lambda) - (\mathrm{Re}(\lambda))^2} \leq -\frac{\sqrt{3}}{2}\,\mathrm{tr}(Q). \tag{2.4}$$

Let us write $r = -\,\mathrm{tr}(Q)$. Since Q is a rate matrix, we have that $\widetilde{Q} = Q + rId_n$ is a non-negative matrix with rows summing to r.

Therefore, $\widetilde{Q}/r$ is a Markov matrix and hence we derive from Proposition 1.2.5 that any eigenvalue $\widetilde{\lambda} \in \sigma(\widetilde{Q})$ satisfies $|\widetilde{\lambda}| \leq r$. Now, if λ is an eigenvalue of Q we have that $\lambda + r \in \sigma(\widetilde{Q})$ which implies that $(\mathrm{Re}(\lambda)+r)^2 + \mathrm{Im}(\lambda)^2 = |\lambda + r|^2$ is upper bounded by r^2. From this we obtain

$$|\operatorname{Im}(\lambda)| \leq \sqrt{r^2 - (\operatorname{Re}(\lambda)+r)^2} = \sqrt{2\ \operatorname{Re}(\lambda)\ \operatorname{tr}(Q) - \operatorname{Re}(\lambda)^2}. \quad (2.5)$$

Since $-r/2 \leq \mathrm{Re}(\lambda)$ by 2.1.3), we have that $r/2 \leq r + \mathrm{Re}(\lambda)$. The remaining inequality in (2.4) follows by using this in (2.5). Indeed:

$$|\operatorname{Im}(\lambda)| \leq \sqrt{r^2 - (\operatorname{Re}(\lambda)+r)^2} \leq \sqrt{r^2 - (r/2)^2} = \sqrt{3r^2/4}.$$

We prove now that

$$|\operatorname{Im}(\lambda)| \leq -\frac{\operatorname{Re}(\lambda)}{\tan(\pi/n)} \leq -\frac{\operatorname{tr}(Q)}{2\tan(\pi/n)} \quad (2.6)$$

for any non-real eigenvalue λ of Q. If $n < 3$, then Q has no complex eigenvalues because 0 is an eigenvalue of any rate matrix and the other root of the characteristic polynomial has to be real as well. Conversely, if $n \geq 3$, the first inequality in (2.6) is obtained by using that

$$|\operatorname{Im}(\lambda)| = |\tan(\operatorname{Arg}\lambda)\operatorname{Re}(\lambda)| = -\operatorname{Re}(\lambda)|\tan(\operatorname{Arg}\lambda)|,$$

the boundary on $|\operatorname{Arg}(\lambda)|$ given in (2.2) and that the modulus of the tangent function restricted to $(-\pi, -\frac{\pi}{2} - \frac{\pi}{n}] \cup [\frac{\pi}{2} + \frac{\pi}{n}, \pi]$ attains its maximum at

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

The second inequality follows by using $-\operatorname{Re}(\lambda) \leq -\operatorname{tr}(Q)/2$, which was proven in the first part of the proof.

From the first inequality in both (2.4) and (2.6) we have $|\operatorname{Im}(\lambda)| \leq b_n(\lambda)$ whereas $b_n(\lambda) \leq B_n$ follows from the definition of $b_n(\lambda)$ and the second inequality of (2.4) and (2.6). □

Remark 2.1.4. Note that for $n \geq 2$ we have $\tan(\pi/n) > \tan(\pi/(n+1))$. Moreover, for $n = 6$ we have $-\frac{\operatorname{tr}(Q)}{2\tan(\pi/n)} = -\frac{\sqrt{3}}{2}\operatorname{tr}(Q)$. Therefore, we have:

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

Similarly, for $n \leq 6$ we have $b_n(\lambda) = -\frac{\operatorname{Re}(\lambda)}{\tan(\pi/n)}$. Indeed, if $n \in \{3,4,5,6\}$ then

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

Figure 2.1 illustrates the statement of Lemma 2.1.3 for different values of n.

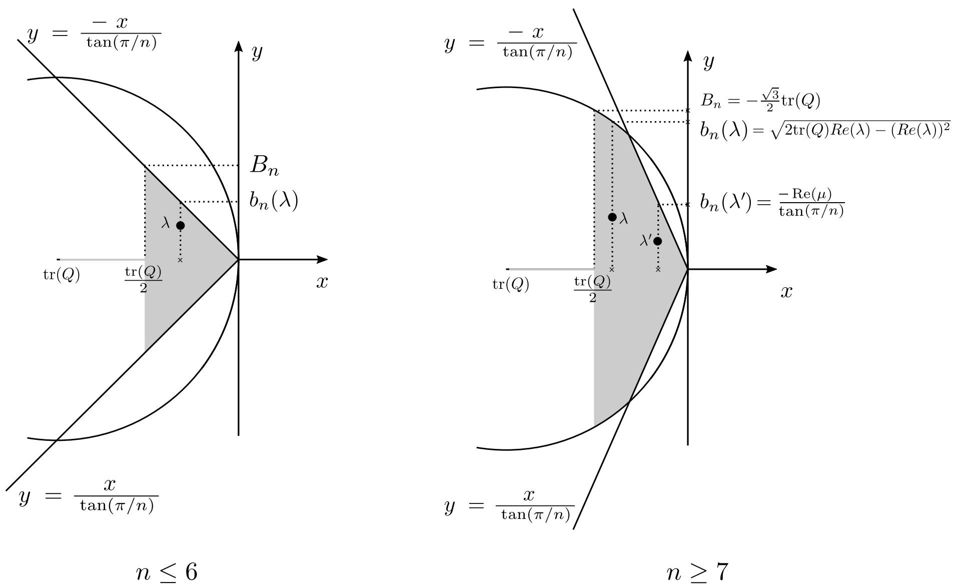

Figure 2.1: Complex region containing the eigenvalues of $n \times n$ rate matrices (Lemma 2.1.3). The two situations in Remark 2.1.4 are represented.

2.2 SUFFICIENT CONDITIONS FOR EMBEDDABILITY AND IDENTIFIABILITY OF RATES

The set of $n \times n$ Markov matrices with different eigenvalues is a dense subset within the set of Markov matrices of size n. If the eigenvalues of such a matrix are real, then there is at most one generator and the embeddability can be decided by computing the unique candidate, the principal logarithm (see Corollary 1.3.8). However, this is not the case if M has non-real eigenvalues.

Lemma 2.2.1. *Let Q be a rate matrix with no null entries and with either a repeated eigenvalue μ or a pair of conjugated complex eigenvalues $\mu, \overline{\mu}$. Then, there exist $t_0 \in \mathbb{R}_{>0}$ such that $M(t) := \exp(Qt)$ is an embeddable matrix whose rates are not identifiable for any $t \geq t_0$.*

Proof. For ease of reading, we write the proof only for the case that Q diagonalizes (if Q does not diagonalize, the proof can be adapted). Under the assumptions of the lemma, we can write

$$Q = P\,\mathrm{diag}(0, \lambda_1, \dots, \lambda_{n-3}, \mu, \overline{\mu})\ P^{-1}$$

for some $P \in GL_n(\mathbb{C})$, $\lambda_1, \dots, \lambda_{n-3} \in \mathbb{C}$. Let us define the matrix $V = P\,\mathrm{diag}(0, \dots, 0, 2\pi i, -2\pi i)\ P^{-1}$. Note that V is a logarithm of Id_n (see Example 1.1.23) that commutes with Q and has row sums equal to zero. Therefore, Proposition 1.1.14 yields that $\exp(tQ + V) = \exp(tQ)\exp(V) = \exp(tQ)$ for all $t \in \mathbb{R}$. As noted earlier in Remark 1.2.13, tQ is a rate matrix for all $t \geq 0$. Since the entries of V are fixed and no entry of Q is equal to zero we derive that for $t > 0$ large enough $Q' = Qt + V$ is a rate matrix satisfying $\exp(Qt) = \exp(Q')$. ☐

Therefore, under the assumptions of the previous lemma if the homogeneous continuous-time Markov process ruled by Q runs for enough time, then its instantaneous rates will stop being identifiable. This can be translated in terms of the determinant of the transiton matrix $M(t) = \exp(Qt)$. For example, Theorem 1.3.10 ii) yields that all embeddable Markov matrices with determinant greater than $e^{-\pi}$ have identifible rates (which are given by the principal logarithm). In the following corollary we use the results from the previous section to relax this constraint on the determinant.

Corollary 2.2.2. *Let M be an $n \times n$ Markov matrix such that* $\det(M) > \min\left\{e^{-\frac{2\pi}{\sqrt{3}}}, e^{-2\pi\tan(\pi/n)}\right\}$. *Then, the unique possible Markov generator of M is* $\mathrm{Log}(M)$. *In particular, M is embeddable if and only if* $\mathrm{Log}(M)$ *is a rate matrix.*

Proof. If Q is a Markov generator of M then $\mathrm{tr}(Q) = \log(\det(M))$ by Proposition 1.1.16. By hypothesis, we have that $\mathrm{tr}(Q)$ is strictly greater than $\min\left\{-\frac{2\pi}{\sqrt{3}}, -2\pi\tan(\pi/n)\right\}$. In this case, Lemma 2.1.3 yields that $|\operatorname{Im}(\lambda)| \leq B_n < \pi$ for any $\lambda \in \sigma(Q)$. Hence, the eigenvalues of Q are the principal logarithm of the eigenvalues of M (see Remark 1.3.2) and Q is necessarily the principal logarithm of M by Corollary 1.1.27. □

Table 2.1 compares the bounds of Corollary 2.2.2 with other previously known bounds for several sizes of Markov matrices.

Matrix size	[Cut73]	[IRW01]	$e^{-2\pi/\sqrt{3}}$	$e^{-2\pi\tan(\pi/n)}$
$n=3$	0.043214	0.5	0.026580	**0.000019**
$n=4$	0.043214	0.5	0.026580	**0.001867**
$n=5$	0.043214	0.5	0.026580	**0.010410**
$n=6$	0.043214	0.5	**0.026580**	**0.026580**
$n=7$	0.043214	0.5	**0.026580**	0.048518

Table 2.1: Lower bounds on the determinant (rounded to the 6th decimal) that allow the characterization of the embeddability in terms of the principal logarithm. In these cases, rate identifiability is also guaranteed. For each size, the lowest bounds appear in boldface.

The next example shows that the bound on the determinant given in Corollary 2.2.2 is sharp for $n = 3$.

Example 2.2.3. Consider the matrices:

$$M = \frac{1}{3}\begin{pmatrix} 1-2e^{-\pi\sqrt{3}} & 1+e^{-\pi\sqrt{3}} & 1+e^{-\pi\sqrt{3}} \\ 1+e^{-\pi\sqrt{3}} & 1-2e^{-\pi\sqrt{3}} & 1+e^{-\pi\sqrt{3}} \\ 1+e^{-\pi\sqrt{3}}+1 & 1+e^{-\pi\sqrt{3}} & 1-2e^{-\pi\sqrt{3}} \end{pmatrix}$$

and

$$P = \begin{pmatrix} 1 & 2\pi\sqrt{3} & 2\pi\sqrt{3} \\ 1 & -\pi\sqrt{3}-3\pi i & -\pi\sqrt{3}+3\pi i \\ 1 & -\pi\sqrt{3}+3\pi i & -\pi\sqrt{3}-3\pi i \end{pmatrix}.$$

It is immediate to check that $P^{-1}MP = \operatorname{diag}(1, -e^{-\pi\sqrt{3}}, -e^{-\pi\sqrt{3}})$. Hence, Theorem 1.1.24 guarantees that the following matrices are logarithms of M:

$$\begin{aligned} Q_1 &= P \operatorname{diag}(\log(1), \log(-e^{-\pi\sqrt{3}}), \log_{-1}(-e^{-\pi\sqrt{3}}))\ P^{-1} \\ &= P \operatorname{diag}(0, -\pi\sqrt{3}+\pi i, -\pi\sqrt{3}-\pi i)\ P^{-1} = \frac{1}{\sqrt{3}} \begin{pmatrix} -2\pi & 0 & 2\pi \\ 2\pi & -2\pi & 0 \\ 0 & 2\pi & -2\pi \end{pmatrix} \end{aligned}$$

$$\begin{aligned} Q_2 &= P \operatorname{diag}(\log(1), \log_{-1}(-e^{-\pi\sqrt{3}}), \log(-e^{-\pi\sqrt{3}}))\ P^{-1} \\ &= P \operatorname{diag}(0, -\pi\sqrt{3}-\pi i, +\pi\sqrt{3}-\pi i)\ P^{-1} = \frac{1}{\sqrt{3}} \begin{pmatrix} -2\pi & 2\pi & 0 \\ 0 & -2\pi & 2\pi \\ 2\pi & 0 & -2\pi \end{pmatrix} \end{aligned}$$

Since both Q_1 and Q_2 are rate matrices, M is embeddable and has at least two Markov generators. Since $\det(M) = e^{-2\pi \tan(\pi/3)} \leq e^{-2\pi/\sqrt{3}}$, we deduce that the bound in Corollary 2.2.2 is sharp for $n = 3$.

Remark 2.2.4. This example can be extended to larger values of n to obtain embeddable matrices $\widetilde{M}$ whose rates are not identifiable and such that $\det(\widetilde{M}) = e^{-2\pi \tan(\pi/3)}$. Fixed $n \geq 4$, this can be done by considering the matrices $\widetilde{M} = \operatorname{diag}(Id_{n-3}, M)$, $\widetilde{Q_1} = \operatorname{diag}(0, Q_1)$ and $\widetilde{Q_2} = \operatorname{diag}(0, Q_2)$ where M, Q_1 and Q_2 are the matrices in example 2.2.3 and 0 is the zero matrix of size $n-3$. In this case, we have that $\exp(\widetilde{Q_i}) = \widetilde{M}$ for $i = 1, 2$ (see Remark 1.1.8). Therefore, $\widetilde{M}$ is an embeddable Markov matrices with $\det(\widetilde{M}) = e^{-2\pi \tan(\pi/3)}$ and at least two Markov generators, namely $\widetilde{Q_1}$ and $\widetilde{Q_2}$.

The bound in Corollary 2.2.2 arises from B_n in Lemma 2.1.3. Hence, a more relaxed hypothesis, which depends not only on the determinant of M but also on its eigenvalues, can be obtained by using $\max_{\lambda \in \sigma(M)} b_n(\log|\lambda|)$

instead of B_n. In order to simplify the notation, given a non-singular Markov matrix M and an eigenvalue $z \in \sigma(M)$ we define

$$\beta_n(z) := \min \left\{ \sqrt{2\log(\det(M))\log|z| - \log^2|z|}, -\frac{\log|z|}{\tan(\pi/n)} \right\}. \tag{2.7}$$

Note that $\beta_n(z)$ is well defined. Indeed, since Markov matrices have real determinant and the modulus of its eigenvalues is bounded by 1 (see Proposition 1.2.5) we have

$$\sqrt{2\log(\det(M))\log|z| - \log^2|z|} \in \mathbb{R}.$$

Moreover, if Q is a Markov generator of M then $\log_k(z) \in \sigma(Q)$ for some $k \in \mathbb{Z}$ (see Remark 1.3.2). In this case, we have $\beta_n(z) = b_n(\log_k(z))$ because $\mathrm{Re}(\log_k(z)) = \log|z|$.

Theorem 2.2.5. *Let M be an $n \times n$ diagonalizable Markov matrix and let Λ be the set formed by its non-real eigenvalues and its eigenvalues with multiplicity ≥ 2. If $\beta_n(z) < \pi$ for all $z \in \Lambda$, then the unique possible Markov generator of M is $\mathrm{Log}(M)$. In particular, M is embeddable if and only if $\mathrm{Log}(M)$ is a rate matrix.*

Proof. If $\Lambda = \emptyset$, then M has pairwise different real eigenvalues and the claim is true by Corollary 1.3.8. If $\Lambda \neq \emptyset$, assume that Q is a Markov generator of M. If $\lambda \in \sigma(Q)$ is real, then e^λ is an eigenvalue of M (see Lemma 1.1.12). In this case, e^λ is real and λ is necessarily its principal logarithm. Now, assume that λ is a non-real eigenvalue of Q. Since Q is real we have that $\overline{\lambda} \in \sigma(Q)$. Moreover, according to Lemma 1.1.12, we have that $e^\lambda, e^{\overline{\lambda}} \in \sigma(M)$. Note that if $e^\lambda \in \mathbb{R}$ then $e^{\overline{\lambda}} = e^\lambda$. Thus, either $z := e^\lambda$ is non-real or it is real and repeated. In any case, we have $z \in \Lambda$. Now, it follows from Theorem 1.1.24 that $\lambda = \log_k(z)$ for some $k \in \mathbb{Z}$ and hence $\mathrm{Re}(\lambda) = log|z|$. From Lemma 2.1.3 we obtain $|\mathrm{Im}(\lambda)| \leq b_n(\lambda) = \beta(z)$ and by hypothesis this is smaller than π for any $z \in \Lambda$. Hence, $\lambda = \log(z)$ and we deduce that all the eigenvalues of Q are principal logarithms of an eigenvalue of M. Thus, $Q = \mathrm{Log}(M)$ by Corollary 1.1.27. □

Remark 2.2.6. Example 2.2.3 together with Remark 2.2.4 show that for any size n there is an embedabble matrix with at least two different Markov generators satisfying $\max_{z\in\Lambda} \beta_n(z) = \pi$. Thus, the hypothesis of Theorem 2.2.5 *can not* be relaxed. Moreover, Theorem 2.2.5 relaxes the hypothesis of Corollary 2.2.2. Indeed, assume that M is a Markov matrix such that $\det(M) > \min\left\{e^{-\frac{2\pi}{\sqrt{3}}}, e^{-2\pi\tan(\pi/n)}\right\}$. As shown in the proof of Corollary 2.2.2 this implies that if Q is Markov generator of M, then $Q = \mathrm{Log}(M)$. Therefore, by Lemma 2.1.3 we have $b_n(\lambda) \leq B_n < \pi$ for any $\lambda \in \sigma(Q)$. Hence, M satisfies the hypotheses of Theorem 2.2.5 because $\beta_n(e^\lambda) = b_n(\lambda)$.

2.3 BOUNDS ON THE NUMBER OF MARKOV GENERATORS

In this section we deal with the embedding problem for $n\times n$ Markov matrices with *pairwise different* eigenvalues, real or not. According to Corollary 1.3.8, if all the eigenvalues of such a matrix are *real*, then its embeddability is determined by the principal logarithm. Although any Markov matrix with non-real eigenvalues has infinitely many real logarithms with rows summing to 0, we will show that only a finite number of them have non-negative off-diagonal entries (Theorem 2.3.3). In this way we are able to design an algorithm that returns all the Markov generators of a Markov matrix with distinct eigenvalues (see Algorithm 2.3.5).

It is well known that a Markov matrix with a non-repeated negative eigenvalue has no Markov generator (Proposition 1.3.6). Because of this and Proposition 1.2.5 i), the real eigenvalues of an embeddable Markov matrix with pairwise different eigenvalues lie in $(0,1]$. Throughout this section we fix an $n\times n$ Markov matrix M with pairwise different eigenvalues and whose real eigenvalues lie in $(0,1]$. Equivalently,

$$M = P\,\mathrm{diag}\big(1, \lambda_1, \dots, \lambda_t, \mu_1, \overline{\mu_1}, \dots, \mu_s, \overline{\mu_s}\big)\; P^{-1} \tag{2.8}$$

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

Definition 2.3.1. Given a Markov matrix M as in (2.8) and $k_1,\dots,k_s \in \mathbb{Z}$, we define $\mathrm{Log}_{k_1,\dots,k_s}(M)$ as the following matrix:

$$P\,\mathrm{diag}\Big(0, \log(\lambda_1), \dots, \log(\lambda_t), \log_{k_1}(\mu_1), \overline{\log_{k_1}(\mu_1)}, \dots, \log_{k_s}(\mu_s), \overline{\log_{k_s}(\mu_s)}\Big)\; P^{-1}.$$

Note that $\mathrm{Log}_{0,\dots,0}(M)$ is the principal logarithm of M, $\mathrm{Log}(M)$ (see Corollary 1.1.27). The next result claims that all real logarithms of M with rows summing to 0 are of this type.

Proposition 2.3.2. *Let M be a Markov matrix as in (2.8). Then, a matrix Q with rows summing to 0 is a real logarithm of M if and only if $Q = \mathrm{Log}_{k_1,\dots,k_s}(M)$ for some $k_1, \dots, k_s \in \mathbb{Z}$.*

Proof. The columns of P are eigenvectors of M. Since the rows of M sum to one and M has no repeated eigenvalue, we can assume without loss of generality that the first column is the vector $\mathbf{1}$. Moreover, we can take the columns corresponding to conjugated complex eigenvalues to be conjugated eigenvectors.

$\Leftarrow$) From (1.9) we have that $\overline{\log_k(\mu)} = \log_{-k}(\overline{\mu})$. Hence, Theorem 1.1.24 yields that $\mathrm{Log}_{k_1,\dots,k_s}(M)$ 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 $\mathbf{1}$ and its corresponding eigenvalue is 0. Moreover, the non-real eigenvalues of Q appear in conjugated pairs and the corresponding eigenvectors appearing as column-vectors in P are also conjugated, thus Q is real.

$\Rightarrow$) Let Q be a real logarithm of M with rows summing to 0. Since M has pairwise different eigenvalues, from Theorem 1.1.24 and Remark 1.1.26 we get:

$$Q = P \,\mathrm{diag}\Big(\log_{k_0}(1), \log_{k_1}(\lambda_1), \dots, \log_{k_t}(\lambda_t), \dots \\ \dots, \log_{k_{t+1}}(\mu_1), \log_{k_{t+2}}(\overline{\mu_1}), \dots, \log_{k_{t+2s-1}}(\mu_s), \log_{k_{t+2s}}(\overline{\mu_s}) \Big)\; P^{-1}.$$

Since the rows of Q sum to 0, we get that $k_0 = 0$. Since Q is real and has no repeated eigenvalues we have that $k_1 = k_2 = \dots = k_t = 0$ and also that its non-real eigenvalues appear in conjugated pairs. According to (1.9) this is only satisfied by taking $k_{t+2m} = -k_{t+2m-1}$ for all $m \in \{1, \dots, s\}$. With these values we have $\log_{-k_{t+2m-1}}(\overline{\mu_m}) = \overline{\log_{k_{t+2m-1}}(\mu_m)}$. □

As a byproduct of the proposition above and Lemma 2.1.3, the next theorem shows that for any Markov matrix with pairwise different eigenvalues there is a finite number of matrices that are candidates to be Markov generators. Therefore, its embeddability can be determined by checking whether a finite family of matrices contains a rate matrix.

Theorem 2.3.3. *If M is a Markov matrix as in (2.8) and $\beta(\mu_i)$ is defined as in (2.7), then*

i) M is embeddable if and only if $\mathrm{Log}_{k_1,\dots,k_s}(M)$ is a rate matrix for some $(k_1,\dots,k_s)\in\mathbb{Z}^s$ satisfying $\left\lceil \frac{-\mathrm{Arg}(\mu_j)-\beta_n(\mu_j)}{2\pi}\right\rceil \le k_j \le \left\lfloor \frac{-\mathrm{Arg}(\mu_j)+\beta_n(\mu_j)}{2\pi}\right\rfloor$ for $j=1,\dots,s$.

ii) M has at most $\prod_j \left\lfloor 1+\frac{\beta_n(\mu_j)}{\pi}\right\rfloor$ Markov generators.

iii) M has at most $\left\lfloor 1-\frac{\sqrt{3}\log(\det(M))}{2\pi}\right\rfloor^s$ Markov generators if $n>6$, at most $\left\lfloor 1-\frac{\log(\det(M))}{2\pi\tan(\pi/n)}\right\rfloor^s$ if $n=3,4,5,6$ and at most one if $n\le 2$.

Proof.

i) According to Proposition 2.3.2, any Markov generator of M can be written as $Q=\mathrm{Log}_{k_1,\dots,k_s}(M)$ for some $k_1,\dots,k_s\in\mathbb{Z}$. In this case, $|\operatorname{Im}\left(\log_{k_j}(\mu_j)\right)|\le b_n(\log_{k_j}(\mu_j))$ by Lemma 2.1.3. Moreover, we have that $|\operatorname{Im}\left(\log_{k_j}(\mu_j)\right)| = |Arg(\mu_j)+2\pi k_j|$ and $\beta_n(\mu_j)=b_n(\log_{k_j}(\mu_j))$, thus $\beta_n(\mu_j)\ge |Arg(\mu_j)+2\pi k_j|$. Using that $0<\mathrm{Arg}(\mu_j)<\pi$ we get:

$$\beta_n(\mu_j)\ge |Arg(\mu_j)+2\pi k_j| = \begin{cases} Arg(\mu_j)+2\pi k_j & \text{if } k_j\ge 0\\ -Arg(\mu_j)-2\pi k_j & \text{otherwise.}\end{cases}$$

We get the asserted bounds by isolating k_j in the expression above.

ii) If $n<3$ then M has only real eigenvalues and hence its only possible Markov generator is $\mathrm{Log}(M)$. For other values of n, it follows from the first statement that if $\mathrm{Log}_{k_1,\dots,k_s}(M)$ is a Markov generator, then k_j lies in a closed interval of length $\frac{\beta_n(\mu_j)}{\pi}$. Since $k_j\in\mathbb{Z}$ for all j we get that M has at most $\prod_j \left\lfloor 1+\frac{\beta_n(\mu_j)}{\pi}\right\rfloor$ generators.

iii) Let us recall that if Q is a Markov generator of M and $\log_k(\mu_j)$ is an eigenvalue of Q then $\beta_n(\mu_j) = b_n(\log_k(\mu_j))$. Hence, by Lemma 2.1.3 and Remark 2.1.4 we have

$$\beta_n(\mu_j) \leq B_n = \begin{cases} -\frac{\log(\det(M))}{2\tan(\pi/n)} & \text{if } n = 3,4,5,6 \\ -\frac{\sqrt{3}}{2}\log(\det(M)) & \text{if } n > 6. \end{cases}$$

The statement follows from this inequality and ii). □

Remark 2.3.4. Theorem 2.2.5 and Corollary 2.2.2 are particular cases of Theorem 2.3.3 obtained by using the bounds given in ii) and iii) respectively. Actually, analogously to Remark 2.2.6, the bound for the number of Markov generators of M given by ii) is more accurate that the bound given by iii). However, the later is much easier to obtain because it does not require to compute of the eigenvalues of M. Moreover, this bound might be related to the expected number of substitutions along the Markov process ruled by M (see section 1.4.2 or [BH87]).

2.3.1 Computational solution to the embedding problem

We finish this chapter by presenting an algorithm which determines the embeddability of a Markov matrix with pairwise different eigenvalues and returns all its Markov generators. The algorithm computes all the logarithms of M described in Theorem 2.3.3 i) and tests if they are rate matrices.

Algorithm 2.3.5 (Markov generators for $n \times n$ matrices with different 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
    $s = \frac{\#\text{non-real eigenvalues}}{2}$ *($\mu_1, \dots, \mu_s$, non-real eigenvalues with $Im(\mu_j) > 0$)*
    if $s > 0$ *(i.e. M has a non-real eigenvalue)* **then**
        for $j = 1, \dots, s$ **do**
            set $l_j = \left\lfloor \frac{-Arg(\mu_j) - \beta_n(\mu_j)}{2\pi} \right\rfloor$ *and* $u_j = \left\lfloor \frac{-Arg(\mu_j) + \beta_n(\mu_j)}{2\pi} \right\rfloor$
        for $k_1 = l_i, \dots, u_i,\ i = 1, \dots, s$ **do**
            compute $\mathrm{Log}_{k_1,\dots,k_s}(M)$
            if $\mathrm{Log}_{k_1,\dots,k_s}(M)$ *is a rate matrix* **then**
                add $\mathrm{Log}_{k_1,\dots,k_s}(M)$ *to generators*
    else
        if $\mathrm{Log}(M)$ *is a rate matrix* **then**
            add $\mathrm{Log}(M)$ *to generators*
    if *generators=[ ]* **then**
        return *"M not embeddable"*
    else
        return *generators*

Remark 2.3.6. As stated in Corollary 2.2.2, if M has a Markov generator different than $\mathrm{Log}(M)$, 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.

3

CHARACTERIZATION OF EMBEDDABLE 4×4 MARKOV MATRICES

In this chapter we solve the embedding problem for any 4×4 Markov matrix. For matrices with different eigenvalues, real or not, we provide a refined version of Theorem 2.3.3 and we give a criterion for the embeddability (Corollary 3.1.7). We also study the embeddability of 4×4 Markov matrices that do not diagonalize or that have repeated eigenvalues.

In the first section of this chapter we present the main results, which solve the embedding problem for 4×4 Markov matrices. In the second section we present algorithms for testing the embeddability of 4×4 diagonalizable matrices. In the third section we discuss the consequences of our results from the perspective of the rate identifiability for 4×4 embeddable matrices.

3.1 EMBEDDABILITY OF 4×4 MARKOV MATRICES

We start by enumerating all possible diagonal forms of a diagonalizable 4×4 Markov matrix with real logarithms (up to ordering the eigenvalues).

Lemma 3.1.1. *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	$\mathrm{diag}(1, \lambda_1, \lambda_2, \lambda_3)$	*with* $\lambda_1, \lambda_2, \lambda_3 \in (0, 1]$ *pairwise different.*
Case II	$\mathrm{diag}(1, \lambda, \mu, \bar{\mu})$	*with* $\lambda \in (0, 1]$, $\mu, \bar{\mu} \in \mathbb{C} \setminus \mathbb{R}$, $\mathrm{Im}(\mu) > 0$.
Case III	$\mathrm{diag}(1, \lambda, \mu, \mu)$	*with* $\lambda \in (0, 1]$, $\mu \in [-1, 1)$, $\mu \neq 0$, $\mu \neq \lambda$.
Case IV	$\mathrm{diag}(1, \lambda, \lambda, \lambda)$	*with* $\lambda \in (0, 1]$.

Proof. First note that M is non-singular (Proposition 1.3.6). Moreover, $|\lambda| \leq 1$ for any $\lambda \in \sigma(M)$ and $\mathbf{1}$ is an eigenvector of M with eigenvalue 1 (Proposition 1.2.5). Hence, if M has a negative eigenvalue, it must have multiplicity 2 by Proposition 1.3.6. Thus, M has no other negative eigenvalue. Similarly, the non-real eigenvalues of M come in conjugated pairs because M is real and hence there is at most one conjugated pair of eigenvalues (and the remaining eigenvalue must be 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 $M - Id$ would be a rank 1 real matrix whose rows sum to 0, which contradicts the fact that $M - Id$ has no negative entries outside the diagonal. This implies that any diagonalizable 4×4 Markov matrix with a real logarithm lies in one of the cases in Lemma 3.1.1. $\square$

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

3.1.1 Case I

The embeddability of Markov matrices when all the eigenvalues are real and different is already solved by Corollary 1.3.8. That result also shows that in this case the rates are identifiable. However, in Case I, we also consider the possibility that the eigenvalue 1 has multiplicity 2. Our next result shows that Corollary 1.3.8 does still hold in this case.

Lemma 3.1.2. *Let $M = P\text{diag}(1, \lambda_1, \lambda_2, \lambda_3)P^{-1}$ be a Markov matrix with $\lambda_1, \lambda_2, \lambda_3 \in (0, 1]$ pairwise different 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 unique Markov generator of M.*

Proof. If $\lambda_1, \lambda_2, \lambda_3$ are different than 1, the embeddability of this case is already solved by Corollary 1.3.8. Otherwise, we can assume $\lambda_1 = 1$ without loss of generality. Under this assumption, let Q be a Markov generator of M. By Lemma 1.1.12, 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 zero because non-real eigenvalues of

Q must appear in conjugated 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 $k_3 = k_4 = 0$. Hence, Corollary 1.1.27 implies that $Q = \mathrm{Log}(M)$. □

3.1.2 Case II

Markov matrices M in Case II (see Lemma 3.1.1) have non-real eigenvalues and an eigendecomposition as $M = P\ \mathrm{diag}(1, \lambda, \mu, \overline{\mu})\ P^{-1}$ with $\lambda \in (0, 1], \mu \in \mathbb{C} \setminus \mathbb{R},\ \mathrm{Im}(\mu) > 0,$ and $P \in GL_4(\mathbb{C})$.

If $\lambda \neq 1$, Proposition 2.3.2 yields that the Markov generators of M are necessarily of the form

$$\begin{aligned} \mathrm{Log}_k(M) &:= P\ \mathrm{diag}\big(0, \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)}\big) P^{-1} \\ &= P\ \mathrm{diag}\big(0, \log(\lambda), \log(\mu) + 2\pi k i, \overline{\log(\mu)} - 2\pi k i\big)\ P^{-1}, \end{aligned} \tag{3.1}$$

for some $k \in \mathbb{Z}$. Note that $\mathrm{Log}_k(M)$ is not the same than the spectral resolution of the $k-$th determinantion of the logarithm in M, which would be denoted as $\log_k(M)$.

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

Proposition 3.1.3. *Let M be a Markov matrix with an eigendecomposition $P\ \mathrm{diag}(1, 1, \mu, \bar{\mu})\ P^{-1}$ with $P \in GL_4(\mathbb{C})$ and $\mu, \bar{\mu} \in \mathbb{C}$ such that $\mu \neq 0$ and $\mathrm{Im}(\mu) > 0$.*

i) If $\widetilde{P}\ \mathrm{diag}(1, 1, \mu, \bar{\mu})\ \widetilde{P}^{-1}$ is another eigendecomposition of M, then

$$P\ \mathrm{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})\ P^{-1} = \widetilde{P}\ \mathrm{diag}(0, 0, \log_k(\mu), \overline{\log_k(\mu)})\ \widetilde{P}^{-1}$$

for any $k \in \mathbb{Z}$. In particular, $\mathrm{Log}_k(M)$ does not depend on the choice of the transformation matrix.

ii) A matrix Q is a real logarithm of M with rows summing to 0 if and only if $Q = \mathrm{Log}_k(M)$ for some $k \in \mathbb{Z}$.

Proof.

i) If $\widetilde{P}$ diag$(1,1,\mu,\bar{\mu})$ $\widetilde{P}^{-1}$ is another eigendecomposition of M, we have that $\widetilde{P} = PA$ for some matrix $A \in Comm^*(\text{diag}(1,1,\mu,\bar{\mu}))$ due to Lemma 1.1.4. Moreover, by Proposition 1.1.5 we have that $Comm^*(\text{diag}(1,1,\mu,\bar{\mu})) = Comm^*(\text{diag}(0,0,\log_k(\mu),\overline{\log_k(\mu)}))$ and hence, 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 1.1.24). Since M is a Markov matrix, we have that $\mathbf{1}$ is an eigenvector of M (see Proposition 1.2.5). Hence we can assume that the first column-vector of P is $\mathbf{1}$ and the rows of $\text{Log}_k(M)$ sum to 0.

Conversely, next we prove that any real logarithm Q of M with rows summing to 0 is of the form $\text{Log}_k(M)$. From Theorem 1.1.24 we have that there are $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ and $A \in Comm^*(\text{diag}(1,1,\mu,\bar{\mu}))$ such that

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

Since the rows of Q sum to 0 we get $k_1 = k_2 = 0$ as in the proof of Lemma 3.1.2. As Q is real, we get that $\log_{k_3}(\mu)$ and $\log_{k_4}(\bar{\mu})$ must be conjugated. According to (1.9), this implies $k_4 = -k_3$. From Proposition 1.1.5 we deduce that A commutes with $(0,0,\log_{k_3}(\mu),\overline{\log_{k_3}(\mu)})$ and hence $Q = \text{Log}_{k_3}(M)$. □

Now that we know that all real logarithms in Case II can be expressed as in (3.1), we decompose $\text{Log}_k(M)$ as

$$\text{Log}_k(M) = \text{Log}(M) + k \cdot V \text{ where } V = P\ \text{diag}(0,0,2\pi i,-2\pi i)\ P^{-1}. \quad (3.2)$$

Remark 3.1.4. Since $\text{Log}_k(M)$ does not depend on the choice of the transformation matrix P (see Proposition 3.1.3), we deduce that the matrix V does not depend on the choice of P either.

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

Lemma 3.1.5. *Let* $M = P\ \mathrm{diag}(1,\lambda,\mu,\overline{\mu})\ P^{-1}$ *be a Markov matrix with* $\lambda \in (0,1], \mu \in \mathbb{C}\setminus\mathbb{R},\ \mathrm{Im}(\mu) > 0,$ *and* $P \in GL_4(\mathbb{C})$*. If* $\mathrm{Log}_{k_1}(M)$ *and* $\mathrm{Log}_{k_2}(M)$ *are rate matrices with* $k_1 < k_2$*, then* $\mathrm{Log}_k(M)$ *is a rate matrix for all* $k \in [k_1, k_2]$*.*

Proof. The proof is immediate because the entries of $\mathrm{Log}_k(M) = \mathrm{Log}(M) + k\cdot V$ depend linearly on k and the set of rate matrices is a convex subset of the space of matrices (see Remark 1.2.13). □

Note that we could use Lemma 2.1.3 to bound the values of k for which $\mathrm{Log}_k(M)$ is a Markov generator, as we did in Chapter 2. However, Lemma 3.1.5 allows us to state a precise description of those logarithms of M that are Markov generators (not only giving a necessary condition). We develop this in the following result.

Theorem 3.1.6. *Let* M *be a Markov matrix with eigendecomposition* $M = P\ \mathrm{diag}(1,\lambda,\mu,\overline{\mu})\ P^{-1}$ *for some* $\lambda \in (0,1]$*,* $\mu \in \mathbb{C}\setminus\mathbb{R}$ *with* $\mathrm{Im}(\mu) > 0$ *and* $P \in GL_4(\mathbb{C})$*. Consider the matrix* $V = P\ \mathrm{diag}(0,0,2\pi i,-2\pi i)\ P^{-1}$ *and define*

$$\mathcal{L} := \max_{(i,j):\ i\neq j,\ V_{i,j}>0} \left\lceil -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rceil, \quad \mathcal{U} := \min_{(i,j):\ i\neq j,\ V_{i,j}<0} \left\lfloor -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rfloor$$

and $\mathcal{N} := \{(i,j) : i \neq j,\ V_{i,j} = 0 \text{ and } \mathrm{Log}(M)_{i,j} < 0\}$*.*
Then, $\mathrm{Log}_k(M)$ *is a rate matrix if and only if* $\mathcal{N} = \emptyset$ *and* $\mathcal{L} \leq k \leq \mathcal{U}$*.*

Proof. By (3.2) we have that $\mathrm{Log}_k(M) = \mathrm{Log}(M) + k\cdot V$. Now, assume that there is $k \in \mathbb{Z}$ such that $\mathrm{Log}_k(M)$ is a rate matrix. In this case, $\mathrm{Log}(M)_{i,j} + kV_{i,j} \geq 0$ for all $i \neq j$. Hence:

a) $0 \leq \mathrm{Log}(M)_{i,j}$ for all $i \neq j$ such that $V_{i,j} = 0$. In particular $\mathcal{N} = \emptyset$.

b) $-\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \leq k$ for all $i \neq j$ such that $V_{i,j} > 0$. In particular $\mathcal{L} \leq k$.

c) $-\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \geq k$ for all $i \neq j$ 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 $\mathrm{Log}_k(M)$ is a rate matrix. First, note that the rows of $\mathrm{Log}_k(M)$ sum to 0, as proved in Propositions 2.3.2 and 3.1.3. Now, consider $i \neq j$, then:

a) if $V_{i,j} = 0$ we have $\mathrm{Log}_k(M)_{i,j} = \mathrm{Log}(M)_{i,j}$. Since $\mathcal{N} = \emptyset$ it follows that $\mathrm{Log}(M)_{i,j} \geq 0$, so $\mathrm{Log}_k(M)_{i,j} \geq 0$.

b) if $V_{i,j} > 0$, then $\mathrm{Log}_k(M)_{i,j} \geq \mathrm{Log}(M)_{i,j} + \mathcal{L} \cdot V_{i,j} \geq \mathrm{Log}(M)_{i,j} + \frac{-\mathrm{Log}(M)_{i,j}}{V_{i,j}} V_{i,j} = 0$.

c) if $V_{i,j} < 0$, then $-\mathrm{Log}_k(M)_{i,j} \leq -\mathrm{Log}(M)_{i,j} - \mathcal{U} \cdot V_{i,j} \leq -\mathrm{Log}(M)_{i,j} - \frac{-\mathrm{Log}(M)_{i,j}}{V_{i,j}} V_{i,j} = 0$. □

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

Corollary 3.1.7. *Let M be a Markov matrix with eigendecomposition $M = P\ \mathrm{diag}(1, \lambda, \mu, \bar{\mu})\ P^{-1}$ with $P \in GL_4(\mathbb{C})$, $\lambda \in (0, 1]$ and $\mu, \bar{\mu} \in \mathbb{C} \setminus \mathbb{R}$. Let $\mathcal{L}$, $\mathcal{U}$ and $\mathcal{N}$ be as in Theorem 3.1.6. Then, M is embeddable if and only if $\mathcal{N} = \emptyset$ and $\mathcal{L} \leq \mathcal{U}$.*

3.1.3 Case III

Let M be a Markov matrix as in Case III of Lemma 3.1.1, that is

$$M = P\ \mathrm{diag}(1, \lambda, \mu, \mu)\ P^{-1} \text{ with } \lambda \in (0, 1],\ \mu \in [-1, 1),\ \mu \neq \lambda, 0. \quad (3.3)$$

for some $P \in GL_4(\mathbb{R})$. Note that this can be seen as a limit case of Markov matrices with a conjugated pair of complex eigenvalues (case II) and, similarly to that case, M has infinitely many real logarithms with rows summing to 0. However, one has to be careful when using Theorem 1.1.24 in the current case because M has repeated eigenvalues and hence different choices for the matrix C may lead to different logarithms (see Remark 1.1.26).

Definition 3.1.8. Let M, P, λ and μ as in (3.3). For any $k \in \mathbb{Z}$ and $x, y, z \in \mathbb{R}$, consider the matrices

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

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

$$L_k(x, y, z) = L + (2\pi k + \mathrm{Arg}\,\mu)\ V(x, y, z).$$

Remark 3.1.9. If $\mu > 0$ we have $L_0(x, y, z) = \mathrm{Log}(M)$ for all $(x, y, z) \in \mathbb{R}^3$. For later use, note that

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

As in the previous case, we start by characterizing all the real logarithms of M with rows summing to 0. To this end, we consider the algebraic variety

$$\mathcal{V} = \{(x,y,z) \in \mathbb{R}^3 \mid xz - y^2 = 1\}. \tag{3.4}$$

$\mathcal{V}$ 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 next theorem shows that the logarithms of M with real entries and rows summing to 0 are of the form $L_k(x, y, z)$ with $(x, y, z) \in \mathcal{V}$. Furthermore, the restriction of $L_k(x, y, z)$ to one of the components of $\mathcal{V}$ parametrizes the real logarithms of M with rows summing to 0.

Theorem 3.1.10. *Let M be a Markov matrix as in (3.3). Then, the following are equivalent:*

i) Q is a real logarithm of M with rows summing to 0.

ii) $Q = L_k(x, y, z)$ for some $(x, y, z) \in \mathcal{V}$, $k \in \mathbb{Z}$.

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

Proof. We first prove that *i*) implies *ii*). We know by Theorem 1.1.24 that any logarithm Q of M can be written as

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

for some $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ and some $C \in Comm^*(\mathrm{diag}(1, \lambda, \mu, \mu))$.
Since Q is a rate matrix we have that 0 is one of its eigenvalues (see Remark 1.2.11). Therefore, we deduce that $k_1 = k_2 = 0$ (even if $\lambda = 1$) because non-real eigenvalues of Q must appear in conjugated-pairs. Moreover, $\log_{k_3}(\mu)$ and $\log_{k_4}(\mu))$ are a conjugated pair. According to (1.9), this implies that

$k_4 = -k_3$ if $\mu > 0$ and $k_4 = -k_3 - 1$ if $\mu < 0$. Thus, if we take $k = k_3$, we have

$$Q = P\,C\,\mathrm{diag}(\log(1), \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)})\,C^{-1}\,P^{-1} \tag{3.5}$$

If all the eigenvalues of Q are real, then $\mu > 0$ and $k = 0$. In this case, the eigenvalues of Q are given by the principal logarithm of the respective eigenvalues of M and hence $Q = \mathrm{Log}(M)$ (see Corollary 1.1.27) and we have $Q = L_0(x, y, z)$ for all $(x, y, z) \in \mathcal{V}$. On the other hand, if Q has a conjugated pair of complex eigenvalues $\log|\mu| \pm (2\pi k + \mathrm{Arg}\,\mu)i$, then the third and fourth columns of $P\,C$ must be a conjugated pair of vectors (up to product by a scalar) because non-real eigenvectors of real matrices appear in conjugated pairs. Furthermore, according to (3.3), P is a real matrix. Hence, it is the third and fourth columns of C that are a conjugated pair of vectors (up to product by a scalar). This fact together with the fact that C commutes with $\mathrm{diag}(1, \lambda, \mu, \mu)$ yields that

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

for some $z_1, z_2 \in \mathbb{C}$ and $z, a, b, c, d \in \mathbb{R}$ satisfying $z_1, z_2 \neq 0$ and $ad - bc \neq 0$ because C is a non-singular matrix. Note that we can decompose C as $C = AB$ where:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix} \qquad B = \begin{pmatrix} z_1 & 0 & 0 & 0 \\ 0 & z_2 & 0 & 0 \\ 0 & 0 & 1 & z \\ 0 & 0 & i & -zi \end{pmatrix} \tag{3.6}$$

Now, let us define the matrix

$$\begin{aligned} J &:= B\,\mathrm{diag}\left(0, \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)}\right)\,B^{-1} \\ &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \log(\lambda) & 0 & 0 \\ 0 & 0 & \log|\mu| & 2\pi k + \mathrm{Arg}\,\mu \\ 0 & 0 & -(2\pi k + \mathrm{Arg}\,\mu) & \log|\mu| \end{pmatrix}. \end{aligned}$$

Note that the matrix Q in (3.5) can be written as $Q = PAJA^{-1}P^{-1}$. This together with the fact that $\mathrm{diag}(0, \log(\lambda), \log|\mu|, \log|\mu|)$ commutes with A (see Proposition 1.1.5) implies that $Q = L + (2\pi k + \mathrm{Arg}\,\mu)V$, where

$$L = P \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \log(\lambda) & 0 & 0 \\ 0 & 0 & \log|\mu| & 0 \\ 0 & 0 & 0 & \log|\mu| \end{pmatrix} P^{-1}$$

and

$$V = P\ A \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} A^{-1}\ P^{-1}.$$

In fact, it is straightforward to check that $V = V(x, y, z)$ with

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

Note that these values satisfy $xz - y^2 = 1$ and hence we can write $Q = L_k(x, y, z)$ for some $k \in \mathbb{Z}$ and $(x, y, z) \in \mathcal{V}$.

We prove now that *ii*) implies *i*). We know that $L_k(x, y, z)$ is real and its rows sum to zero by definition. Hence it is enough to check that if $(x, y, z) \in \mathcal{V}$, then $L_k(x, y, z)$ is a logarithm of M. To this end, consider the matrix

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

If $(x, y, z) \in \mathcal{V}$ then we have $x \neq 0$ and $z = \frac{1+y^2}{x}$. In this case, a straightforward computation shows that

$$L_k\left(x, y, \frac{1+y^2}{x}\right) = P(AB)\ \mathrm{diag}\left(0, \log(\lambda), \log_k(\mu), \overline{\log_k(\mu)}\right)\ (AB)^{-1}P^{-1},$$

where B is defined as in (3.6).

According to Proposition 1.1.5, both A and B commute with $\operatorname{diag}(1, \lambda, \mu, \mu)$ and hence so does AB. Therefore, Theorem 1.1.24 yields that $L_k\left(x, y, \frac{1+y^2}{x}\right)$ is a logarithm of M.

We just proved that the real logarithm of M with rows summing to 0 are of the form $Q = L_k(x, y, z)$ for some $k \in \mathbb{Z}$ and $(x, y, z) \in \mathcal{V}$. By Remark 3.1.9, we can take $(x, y, z) \in \mathcal{V}_+$ without loss of generality. To prove that k and (x, y, z) are unique if $Q \neq \operatorname{Log}(M)$, we assume that $L_k(x, y, z) = L_{\widetilde{k}}(\widetilde{x}, \widetilde{y}, \widetilde{z})$ for some $\widetilde{k} \in \mathbb{Z}$ and $(\widetilde{x}, \widetilde{y}, \widetilde{z}) \in \mathcal{V}_+$. In this case, we have

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

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

$$x = \frac{2\pi\widetilde{k} + \operatorname{Arg}\mu}{2\pi k + \operatorname{Arg}\mu}\widetilde{x} \qquad y = \frac{2\pi\widetilde{k} + \operatorname{Arg}\mu}{2\pi k + \operatorname{Arg}\mu}\widetilde{y} \qquad z = \frac{2\pi\widetilde{k} + \operatorname{Arg}\mu}{2\pi k + \operatorname{Arg}\mu}\widetilde{z}.$$

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

Remark 3.1.11. Excluding the case of the principal logarithm, every real logarithm of M with rows summing to 0 can also be realized as some $L_k(x, y, z)$ for a unique $k \in \mathbb{Z}$ and a unique $(x, y, z) \in \mathcal{V}_-$ (see Remark 3.1.9).

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

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

Note that the entries of $L_k(x, y, z)$ 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 3.1.10 we obtain that the set of Markov generators for a matrix in Case III can be described as $\bigcup_k \mathcal{P}_k \cap \mathcal{V}_+$. As a consequence, we have the following embeddability criterion for 4×4 Markov matrices with two repeated eigenvalues.

Corollary 3.1.12. *Let M be a Markov matrix as in (3.3).*

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

$$\lceil \frac{\log(\mu)}{2\pi} \rceil \leq k \leq \lfloor \frac{-\log(\mu)}{2\pi} \rfloor.$$

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

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

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

Proof. Let M be a Markov matrix as in (3.3). We first show that if Q is a Markov generator of M, then $Q = L_k(x, y, z)$ for some $(x, y, z) \in \mathcal{V}_+$ and some $k \in \mathbb{Z}$ satisfying

$$\frac{-\operatorname{Arg}\mu + \log|\mu|}{2\pi} \leq k \leq \frac{-\operatorname{Arg}\mu - \log|\mu|}{2\pi}. \tag{3.7}$$

Indeed, if Q is a Markov generator of M, then it has at most one conjugated pair of non -real eigenvalues, $\log_k(\mu)$ and $\overline{\log_k(\mu)}$. It follows from Lemma 2.1.3 that their imaginary part $|\operatorname{Im}(\log_k(\mu))| = \operatorname{Arg}(\mu) + 2\pi k$ is bounded by $\beta_4(\mu) = -\log|\mu|$.
Since $k \in \mathbb{Z}$, the bounds on k are a straightforward consequence of (3.7). 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 $\lceil -\frac{1}{2} + \frac{\log|\mu|}{2\pi} \rceil \leq \lfloor -\frac{1}{2} - \frac{\log|\mu|}{2\pi} \rfloor$ if and only if $\log|\mu| < -\pi$. Hence, if $\mu < -e^{-\pi}$ there is no k satisfying the embeddability conditions in the statement. □

Remark 3.1.13. The inequalitiesns in Corollary 3.1.12 are tight. Indeed, for Corollary 3.1.12 i) the equality is obtaned uniquely by $M = Id$. Moreover, we will see in the following chapter an example of an *embeddable* Markov matrix with two repeated eigenvalues (3.3) with $\mu = -e^{-\pi}$ (Example 4.3.2).

3.1.4 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 (see [Ste16, Sec. 7.3.1]). The embeddability of this family of matrices is also studied in [BS20].

Proposition 3.1.14. *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) $\mathrm{Log}(M)$ *is a rate matrix.*

Proof. If $M = Id$, that is $\lambda = 1$, then it follows from Theorem 1.1.24 that $Log(M)$ is the zero matrix and hence it is a Markov generator of M. Moreover, it follows from Corollary 2.2.2 the zero matrix is the only Markov generator of the identity matrix.
Now, let us assume $\lambda \neq 1$. Due to Proposition 1.1.16 we get 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 $\mathrm{Log}(M)$ is a rate matrix.
Since M is diagonalizable, $M - \lambda Id$ is a rank 1 matrix whose rows sum to $1 - \lambda$ (because M is Markov). Hence, M can be written as:

$$M = \begin{pmatrix} a+\lambda & b & c & d \\ a & b+\lambda & c & d \\ a & b & c+\lambda & d \\ a & b & c & d+\lambda \end{pmatrix}, \tag{3.8}$$

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

Let us fix $P \in GL_4(\mathbb{R})$ such that $M = P\,\mathrm{diag}(1,\lambda,\lambda,\lambda)\,P^{-1}$. If $\det(M) > 0$ then $\lambda \in (0,1)$ and $x := \log(\lambda) \in \mathbb{R}_{<0}$. In this case, we have:

$$\begin{aligned} \mathrm{Log}(M) &= P\,\mathrm{diag}(0,x,x,x)\,P^{-1} = x\big(P\,\mathrm{diag}(0,1,1,1)\,P^{-1}\big) \\ &= \frac{x}{\lambda-1}\big(P\,\mathrm{diag}(1,\lambda,\lambda,\lambda)\,P^{-1} - Id\big) = \frac{x}{\lambda-1}(M - Id). \end{aligned}$$

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

Remark 3.1.15. In the context of continuous-time DNA nucleotide substitution models, if a matrix with three repeated eigenvalues is embeddable then it is a transition matrix for the Felsenstein 81 model [Fel81]. The stable distribution of such matrices is given by $\Pi = (a, b, c, d)/(a + b + c + d)$, where a, b, c, d are as in (3.8). When the stable distribution is uniform, that is $a = b = c = d$, we recover the Jukes-Cantor model [JC69].

3.1.5 Non-diagonalizable matrices

If we restrict the embedding problem to non-diagonalizable 4×4 matrices we have:

Theorem 3.1.16. *A non-diagonalizable 4×4 Markov matrix M is embeddable if and only if it has only positive eigenvalues and $\mathrm{Log}(M)$ 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 Markov 4×4 matrix. Thus, M is non-singular and it has no negative eigenvalues. Since the eigenvalue 1 has the same algebraic and geometric multiplicity (see Remark 1.2.6) we deduce that M has at most one Jordan block of size greater than 1×1 and, in this case, its Jordan form is necessarily one of the following (after a suitable reordering of the Jordan blocks):

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda & 1 & 0 \\ 0 & 0 & \lambda & 1 \\ 0 & 0 & 0 & \lambda \end{pmatrix} \text{ with } \lambda \neq 1 \quad \text{or} \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 0 & 0 \\ 0 & 0 & \lambda_2 & 1 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix} \text{ with } \lambda_2 \neq 1.$$

According to Proposition 1.3.6, if M is embeddable then its eigenvalues are necessarily positive. Moreover, if the Jordan form of M has no repeated Jordan blocks, then $\mathrm{Log}(M)$ is the unique real logarithm of M and hence M is embeddable if and only if $\mathrm{Log}(M)$ is a rate matrix. Conversely, if M has a real logarithm other than $\mathrm{Log}(M)$, we deduce that the blocks of any Jordan form of M can be reordered as

$$J := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \lambda & 1 \\ 0 & 0 & 0 & \lambda \end{pmatrix} \text{ with } \lambda \in (0,1).$$

In this case, let P be a Jordan transformation matrix for M for such Jordan form. Since $\lambda > 0$, we obtain from Theorem 1.1.25 that if Q is a logarithm of M then there are $k_1, k_2, k_3 \in \mathbb{Z}$ and $C \in Comm^*(J)$ such that

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

If Q is a rate matrix, it is a real matrix and hence $k_1 = -k_2$ and $k_3 = 0$. Moreover, 0 is an eigenvalue of Q and hence $k_1 = -k_2 = 0$. Therefore, the eigenvalues of Q are the principal logarithms of the eigenvalues of M, so that $Q = \mathrm{Log}(M)$ by Corollary 1.1.27. □

3.2 ALGORITHMS FOR TESTING EMBEDDABILITY

From the results developed in the previous sections we are able to prove that the embeddability of a 4×4 Markov matrix M with different eigenvalues (real or not) can be checked directly by looking at its principal logarithm $\mathrm{Log}(M)$ together with a basis of eigenvectors. We summarize this in the following result.

Theorem 3.2.1. *Let $M = P\mathrm{diag}(1, \lambda_1, \lambda_2, \lambda_3)P^{-1}$ 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 $V = P\ \mathrm{diag}(0, 0, 2\pi i, -2\pi i)\ P^{-1}$ and*

$$\mathcal{L} := \max_{(i,j):\ i\neq j,\ V_{i,j}>0} \left\lceil -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rceil, \quad \mathcal{U} := \min_{(i,j):\ i\neq j,\ V_{i,j}<0} \left\lfloor -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rfloor.$$

Otherwise, write $\mathcal{L} = \mathcal{U} = 0$ and let V denote the 4×4 zero matrix. Set

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

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 $\mathrm{Log}(M) + kV$ with $k \in [\mathcal{L}, \mathcal{U}]$.

Proof. We know that $|\lambda_i| \leq 1$ and, if M is embeddable, $\lambda_i \notin \mathbb{R}_{\leq 0}$ for any $i = 1, 2, 3$ (see Proposition 1.2.5). If all the eigenvalues of M are real, then M lies in Case I of Lemma 3.1.1. In this case, $\mathrm{Log}(M)$ is the only possible Markov generator for M (Lemma 3.1.2). From Proposition 1.2.5 and the definition of principal logarithm we have that $\mathbf{1} = (1, 1, 1, 1)^t$ is an eigenvector of $\mathrm{Log}(M)$ with eigenvalue $\log(1) = 0$ and hence the rows of $\mathrm{Log}(M)$ sum to 0. Therefore, as $V = 0$, we have that $\mathrm{Log}(M)$ is a rate matrix if and only if $\mathcal{N} = \emptyset$. Conversely, if M has a non-real eigenvalue then it lies in Case II of Lemma 3.1.1. In this case, $\mathrm{Log}(M) + kV = \mathrm{Log}_k(M)$ and the claim follows immediately from Theorem 3.1.6 and Corollary 3.1.7. □

According to the previous result, we present an algorithm (Algorithm 3.2.2) that solves both the embedding problem and the rate identifiability problem for 4×4 Markov matrices in Cases I and II. In particular, this algorithm solves the embedding problem for a dense subset of 4×4 Markov matrices. Hence, we can use it to determine how big the set of embeddable Markov matrices is within the set of all Markov matrices and other meaningful sets (see Definition 1.4.11). This is summarized in Table 3.1.

	Samples	Embeddable samples	Proportion of embeddable
Δ	10^7	5774	0.0005774
Δ_{Id}	4998008	5774	0.0011553
Δ_{dlc}	148375	5460	0.0367987
Δ_{dd}	2479	299	0, 1206132

Table 3.1: We sampled 10^7 Markov matrices uniformly and independently from the space of 4×4 Markov matrices Δ. For each of these sets introduced in Definition 1.4.11 (Δ, Δ_{Id}, Δ_{dlc} and Δ_{dd}), the first column shows how many sample points lie in the set, the second column shows how many of them are embeddable and the third column displays the corresponding proportion. Embeddability was checked with Algorithm 3.2.2.

Algorithm 3.2.2.

```
input  : M, a 4×4 Markov matrix with different eigenvalues as in
         Thm 3.2.1.
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 Principal = Log(M)
    if all the eigenvalues are real then
        if Principal is a rate matric then
            add Principal to generators
    else
        compute P and V as in Theorem 3.2.1
        compute ℒ, 𝒰 and 𝒩
        if 𝒩 = ∅ then
            for k ∈ ℤ such that ℒ ≤ k ≤ 𝒰 do
                compute Log_k(M) = Principal + k V
                if Log_k(M) is a rate matric then
                    add Log_k(M) to generators
if generators = [ ] then
    return "M not embeddable"
else
    return generators
```

The previous algorithm can also be used to determine the embeddability of non-diagonalizable matrices and also for diagonalizable matrices in case IV of Lemma 3.1.1, due to the fact that these matrices have real eigenvalues and they are embeddable if and only if their principal logarithm is a rate matrix (see Proposition 3.1.14 and Theorem 3.1.16). However, the embeddability of a matrix with three equal eigenvalues can be determined more easily by checking the sign on its determinant (see Proposition 3.1.14).

From Corollary 3.1.12, we derive the following algorithm to decide the embeddability of Markov matrices in Case III:

Algorithm 3.2.3 (Markov generators of 4×4 matrices with two repeated eigenvalues)**.**

```
input  : M (Markov matrix) and P as in (3.3).
output: One of its Markov generators L_k(x,y,z) for each k ∈ ℤ
        (if they exist).

generators = [ ]
compute the eigenvalues of M: 1, λ, μ, μ
if det(M) > 0 and μ ≥ −e^{−π} then
    Compute L = P diag(0, log(λ), log|μ|, log|μ|) P^{−1}
    set 𝓛 = ⌈(−Arg μ + log|μ|)/(2π)⌉ and 𝓤 = ⌊(−Arg μ − |log(μ)|)/(2π)⌋
    for k ∈ [𝓛,𝓤] ∩ ℤ: do
        if 𝒫_k ∩ 𝒱_+ ≠ ∅ then
            choose (x,y,z) ∈ 𝒫_k ∩ 𝒱_+ (see below)
            add L_k(x,y,z) = L + k V(x,y,z) to generators

if generators = [ ] then
    return "M not embeddable"
else return generators
```

Remark 3.2.4. If $L_k(x,y,z) \neq \mathrm{Log}(M)$ then each choice of $(x,y,z) \in \mathcal{P}_k \cap \mathcal{V}_+$ in the algorithm above would give a different Markov generator of M (see Theorem 3.1.10). 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).

Next, we explain how to find generators for 4×4 Markov matrices with two repeated eigenvalues by using Algorithm 3.2.3. More precisely, we explain how to check whether the intersection $\mathcal{P}_k \cap \mathcal{V}_+$ in Algorithm 3.2.3 is empty or not and how to choose a point in it (if not empty).

Let M be a Markov matrix with eigendecomposition as in (3.3), that is $M = P\ \mathrm{diag}(1, \lambda, \mu, \mu)\ P^{-1}$ with $P \in GL_4(\mathbb{R})$, $\lambda > 0$ and $\mu \in [-1, 1)$ such that $\mu \neq 0$ and $\mu \neq \lambda$. In this case, Theorem 3.1.10 yields that each Markov generator other than $\mathrm{Log}(M)$ can be uniquely expressed as $L_k(x,y,z)$ for some $k \in \mathbb{Z}$ and some $(x,y,z) \in \mathcal{P}_k \cap \mathcal{V}_+$.

Assume that $k=0$ and $\mathrm{Arg}(\mu)=0$. Then, $L_0(x,y,z)$ is 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 $L_k(x,y,z) \neq \mathrm{Log}(M)$. This assumption is equivalent to assuming that $2\pi k + \mathrm{Arg}\,\mu \neq 0$.

We denote by $l_{i,j}$ the entries of the matrix L in Definition 3.1.8 and by $p_{i,j}$ and $\widetilde{p}_{i,j}$ the entries of P and P^{-1} respectively. $\mathcal{P}_k$ is the set of solutions for the system of inequalities $L_k(x,y,z)_{i,j} \geq 0$ for all $i \neq j$, where $L_k(x,y,z) = L + (2\pi k + \mathrm{Arg}\,\mu)V(x,y,z)$. A direct computation shows that the entries of $V(x,y,z)$ depend linearly on x, y and z:

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

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

$$p_{i,3}\widetilde{p}_{4,j}x - p_{i,4}\widetilde{p}_{3,j}z + (p_{i,4}\widetilde{p}_{4,j} - p_{i,3}\widetilde{p}_{3,j})y = \frac{-l_{i,j}}{2\pi k + \mathrm{Arg}\,\mu}. \tag{3.9}$$

It follows from (3.9) that for each $i \neq j$ the faces of the polyhedron $\mathcal{P}_{k_1}$ and $\mathcal{P}_{k_2}$ corresponding to the (i,j)-entry of $L_k(x,y,z)$ are parallel for any $k_1, k_2 \in \mathbb{Z}$.

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 $f(x,y,z)$ in the vertices, edges and faces of $\mathcal{P}_k$ according to the following steps:

Step 1 Evaluate $f(x,y,z)$ on each of the vertices of $\mathcal{P}_k$. If the evaluation of f in all the vertices of $\mathcal{P}_k$ has the same sign (and none is equal to 0), then we proceed to step 2.

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 a valid value for (x, y, z) it is enough to find a point P 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 can chose that vertex itself.

Step 2 Find the roots of $f(x, y, z)$ lying on each edge of $\mathcal{P}_k$. To do so, it is enough to compute the roots of $f(x, y, z)$ in each line containing an edge of $\mathcal{P}_k$ and check whether they lie in the polyhedron or not. If the edges of $\mathcal{P}_k$ do not intersect $\mathcal{V}_+$, then we can look at the faces of $\mathcal{P}_k$ (see the next step).

If we find a simple root or two different roots in one of the edges, we can choose (x, y, z) as one of these roots. In this case, $\mathcal{V}_+$ cuts the interior of $\mathcal{P}_k$ and hence there are infinitely many generators.

If all the roots lying in the edges have multiplicity 2, then we can choose the values of (x, y, z) corresponding to any of these points.

Step 3 For $i \neq j$ consider the intersection $H_{i,j} \cap \mathcal{V}_+ \neq \emptyset$, where $H_{i,j}$ is the plane defined by (3.9). If the intersection is not empty, chose a point in it (see next paragraph) and check whether it belongs to $\mathcal{P}_k$ or not. Note that in the previous step we got that the edges of $\mathcal{P}_k$ do not intersect $\{f(x, y, z) = 0\}$. Hence, if $H_{i,j} \cap \mathcal{V}_+ \neq \emptyset$ then 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 $L_k(x, y, z)$ 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.

Next, we give an insight on how to find $P \in H_{i,j} \cap \mathcal{V}_+$ (if not empty). For ease of reading we write as $Ax + By + Cz = D$ the equation of $H_{i,j}$ (3.9). 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

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

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

i) If $B^2 - 4AC < 0$, compute both roots of $\Delta(x) = 0$. If the roots are non-real or negative then $\mathcal{V}_+ \cap H_{i,j} = \emptyset$. If both roots are real and positive, then all the values between them satisfy $\Delta(x) \geq 0$. Note that, in the current case it is not possible to have one positive root is positive and one negative root because $\mathcal{V} \cap \{x = 0\} = \emptyset$.

ii) If $B^2 - 4AC > 0$, then $\Delta(x) > 0$ when $x \to +\infty$.

iii) If $B^2 - 4AC = 0$ and $CD > 0$, then $\Delta(x) > 0$ when $x \to +\infty$.

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 the intersection of $\mathcal{V}_+$ with the face $H_{i,j}$ is unbounded with respect to x.

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

3.3 RATE IDENTIFIABILITY OF 4 × 4 EMBEDDABLE MARKOV MATRICES

The identifiability of rates for 4 × 4 embeddable matrices has been mainly solved by the previous results of this chapter (see Table 3.2 below, which summarizes these results). Next, we study the missing case of three repeated eigenvalues.

Proposition 3.3.1. *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 unique generator is Log(M).*

Proof. Let Q be a Markov generator of 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 2.1.3 that their imaginary part lies is bounded by $\pm 2\pi$. Since the eigenvalues of M are real and positive this implies that the non-zero eigenvalues of Q are $\log(\lambda)$ and hence $Q = \mathrm{Log}(M)$. □

Remark 3.3.2. We do not know whether $\det(M) > e^{-6\pi}$ is a sharp bound. Note that, it is lower than the bounds given by Corollary 2.2.2 ($\det(M) > e^{-2\pi}$) and by Theorem 2.2.5 ($\det(M) > e^{-3\pi}$). However, the largest determinant of a 4×4 embeddable matrix with three equal eigenvalues and non-identifiable rates that we have been able to find is $e^{-12\pi}$, and corresponds to the matrix

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

Indeed, in addition to its principal logarithm

$$\mathrm{Log}(M) = \begin{pmatrix} -3\pi & \pi & \pi & \pi \\ \pi & -3\pi & \pi & \pi \\ \pi & \pi & -3\pi & \pi \\ \pi & \pi & \pi & -3\pi \end{pmatrix}$$

we have found another six Markov generators for M:

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

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

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

Note that Theorem 2.3.3 bounds the number of generators of a Markov matrix with no repeated eigenvalues. Moreover, Algorithm 2.3.5 lists all the generators of such a matrix. If we restrict the identifiability problem to 4×4 Markov matrices, we were 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 three (Case IV) for which we have Proposition 3.3.1. This is summarized in Table 3.2.

Diagonal form of M	**Embeddability criterion**	**Number of generators**
Case I	$\mathrm{Log}(M)$ is a rate Matrix	One
Case II	$\mathcal{N} = \emptyset$ and $\mathcal{L} \leq \mathcal{U}$ (Cor. 3.1.7)	$\mathcal{U} - \mathcal{L} + 1$ (Thm. 3.1.6)
Case III	$\bigcup_k (\mathcal{P}_k \cap \mathcal{V}) \neq \emptyset$ (Cor 3.1.12)	$\sum_k \#(\mathcal{P}_k \cap \mathcal{V})$ (Rmk. 3.2.4)
Case IV	M is embeddable (Prop. 3.1.14)	One if $\det(M) > e^{-6\pi}$ (Prop. 3.3.1)
M does not diagonalize	$\mathrm{Log}(M)$ is a rate Matrix (Thm. 3.1.16)	One (Thm. 3.1.16)
Other diagonal forms	M is not embeddable	–

Table 3.2: Embeddability criterion and number of generators for a 4×4 Markov matrix depending on its Jordan form. The cases of diagonalizable embeddable matrices (Cases I, II, III and IV) are described in Lemma 3.1.1.

4

THE EMBEDDING PROBLEM FOR KIMURA NUCLEOTIDE SUBSTITUTION MODELS

In this chapter we deal with the embeddability of K3P Markov matrices introduced in section 1.4.1. In terms of modelling, this corresponds to decide which transition matrices within the model have a homogeneous continuous-time realization. Recall that K3P matrices are real and have the form

$$K(a,b,c,d) = \begin{pmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{pmatrix}.$$

When $c = d$ such a matrix is said to be a K2P matrix whereas for $b = c = d$ it is called a JC matrix (see Section 1.4.1).

A key fact for the specialization of the results obtained in Chapter 3 in the setting of K3P Markov matrices is that all K3P matrices are simultaneously diagonalizable through the following Hadamard matrix (see [ES93, HP93]):

$$S := \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \tag{4.1}$$

Note that K3P matrices are symmetric. Thus, by the spectral theorem its eigenvalues are real and we can obtain an orthonormal basis of eigenvectors.

Indeed, $S^2 = 4 \cdot Id$, so $S^{-1} = \frac{1}{4}S$. The following lemma can be proved by direct computation using the matrix S just introduced.

Lemma 4.0.1. *A 4×4 matrix is K3P if and only if it can be diagonalized by S. In this case, $K(a, b, c, d) = S\,D\,S^{-1}$, with $D = \mathrm{diag}(a+b+c+d,\ a+b-c-d, a-b+c-d,\ a-b-c+d)$.*

Remark 4.0.2. If we identify the set of nucleotides $\{\mathtt{A}, \mathtt{G}, \mathtt{C}, \mathtt{T}\}$ with the elements in $\mathbb{Z}_2 \times \mathbb{Z}_2$ and label the rows and columns of a K3P matrix $A = (a_{ij})$ accordingly, then we have that $a_{ij} = a_{kl}$ if and only if $i - j = k - l$ for any $i, j, k, l \in \mathbb{Z}_2 \times \mathbb{Z}_2$. Because of this, the K3P model lies in the class of *group-based models* [SS05]. In this setting the matrix $S^{-1}AS$ is called the *Fourier transform* of the K3P matrix A [ES93].

For the particular case of K3P *Markov* matrices, we have that the eigenvalue $a + b + c + d$ is equal to 1. From this, we derive that every K3P Markov matrix is determined by the other three eigenvalues:

$$\lambda := a + b - c - d, \qquad \mu := a - b + c - d, \qquad \gamma := a - b - c + d. \quad (4.2)$$

Moreover, it is immediate to check that a matrix $M = K(a, b, c, d)$ is K2P (resp. JC) if and only if $\mu = \gamma$ (resp. $\lambda = \mu = \gamma$).

Througout this chapter we will fix the matrix S as in (4.1) and we shall use λ, μ, γ in (4.2) to denote the eigenvalues of $K3P$ matrices.

In the first section of this chapter we study the embedding problem for K3P Markov matrices when we require the Markov generators to be K3P matrices (model-embeddability). In the second section we characterize the set of all embeddable K3P matrices. In the third section we study the identifiability of rates of K3P embeddable matrices with two equal eigenvalues. When restricting the embedding problem and the rate identifiability problem to K3P Markov matrices, the results in the second and third sections in this chapter improve those in Chapter 3. Finally, in the fourth section we compute the volumes of embeddable matrices within some meaningful subsets of transition matrices in the K3P model, including the transition matrices of the K2P model and the JC model.

4.1 MODEL EMBEDDABILITY OF K3P MARKOV MATRICES

When working with phylogenetic trees, one needs that set of transition matrices is multiplicatively closed in order to keep the study and the parameter estimation consistent (see Section 1.4.3). In the continuous-time framework, this leads to the question whether the product of model-embeddable matrices is model-embeddable.

Lemma 4.1.1. *Matrix multiplication is commutative and closed within the set of $K3P$ matrices. Moreover, the product of $K3P$-embeddable matrices is $K3P$-embeddable.*

Proof. We have that $K(a,b,c,d) \cdot K(a',b',c',d') = (S\,D\,S^{-1}) \cdot (S\,D'\,S^{-1}) = S\,DD'\,S^{-1}$, is a K3P matrix by Lemma 4.0.1. Since D and D' are diagonal matrices, we have that $D\,D' = D'\,D$ and from this, the product of K3P matrices is commutative. Therefore, for any K3P rate matrices Q_1 and Q_2, Proposition 1.1.14 yields $\exp(Q_1)\exp(Q_2) = \exp(Q_1 + Q_2)$. To conclude the proof it is enough to note that $Q_1 + Q_2$ is also a K3P rate matrix. □

The model embeddability for K3P matrices has has been largely discussed (and solved) in a more general context [AKK21] (see also [Mat08]). According to the previous lemma, the following characterizes K3P-embeddabable matrices in term of its eigenvalues.

Theorem 4.1.2. *Let M be a K3P Markov matrix with eigenvalues $1, \lambda, \mu, \gamma$. Then, there exists a K3P matrix Q such that $\exp(Q) = M$ if and only if $\lambda, \mu, \gamma > 0$. In this case, Q is necessarily the principal logarithm $Log(M) = S\operatorname{diag}(0, \log(\lambda), log(\mu), \log(\gamma))\ S^{-1}$.*

Proof. First of all, if $\lambda, \mu, \gamma > 0$, then we can take principal logarithms of λ, μ, γ and define Q as the principal logarithm of M, i.e. $Q := Log(M) = S\operatorname{diag}(0, \log(\lambda), \log(\mu), \log(\gamma))\ S^{-1}$. Then, Q is a real matrix, $\exp(Q) = M$ and it has K3P form because of Lemma 4.0.1 and (1.4). Conversely, if Q is a K3P matrix which is also a logarithm of M, then the eigenvalues of Q are real by the spectral theorem for symmetric matrices. Therefore, the eigenvalues of M have to be positive by Lemma 1.1.12. Moreover, by Lemma 4.0.1, Q can be written as $Q' = S\ \operatorname{diag}(r,s,u,v)\ S^{-1}$, for some

$r, s, u, v \in \mathbb{R}$. Because of Lemma 1.1.12, these values are real logarithms of $1, \lambda, \mu, \gamma$. Using that the only real logarithm of a real number is its principal logarithm we derive from Corollary 1.1.27 that Q is necessarily the principal logarithm of M. $\square$

We conclude this section by characterizing when the principal logarithm of a K3P Markov matrix is a Markov generator. Together with the previous theorem, this solves the model embeddability for the K3P model (and its submodels).

Lemma 4.1.3. *Let M be a K3P Markov matrix with eigenvalues $1, \lambda, \mu, \gamma$. Then, $Log(M)$ is a rate matrix if and only if $\lambda, \mu, \gamma > 0$ and*

$$\lambda \geq \mu\gamma, \qquad \mu \geq \lambda\gamma, \qquad \gamma \geq \lambda\mu. \tag{4.3}$$

Proof. Since $\mathrm{Log}(M)$ is a primary logarithm of M it can by diagonalized by S and hence it is a K3P matrix (see Lemma 4.0.1). More precisely, from the definition of principal logarithm and Lemma 4.0.1 we derive that $\mathrm{Log}(M) = K(\widetilde{a}, \widetilde{b}, \widetilde{c}, \widetilde{d})$, where

$$\widetilde{a} = \tfrac{1}{4}\big(log(\lambda) + log(\mu) + log(\gamma)\big), \qquad \widetilde{b} = \tfrac{1}{4}\big(log(\lambda) - log(\mu) - log(\gamma)\big),$$

$$\widetilde{c} = \tfrac{1}{4}\big(log(\mu) - log(\lambda) - log(\gamma)\big), \qquad \widetilde{d} = \tfrac{1}{4}\big(log(\gamma) - log(\lambda) - log(\mu)\big).$$

It is immediate that $\widetilde{a} + \widetilde{b} + \widetilde{c} + \widetilde{d} = 0$. Therefore, we only need to check that the non-diagonal entries $\widetilde{b}$, $\widetilde{c}$ and $\widetilde{d}$ of $Log(M)$ are non-negative if and only if the inequalities (4.3) are satisfied. Indeed,

$$\beta \geq 0 \Leftrightarrow \frac{log(\lambda) - log(\mu) - log(\gamma)}{4} \geq 0 \Leftrightarrow log\left(\frac{\lambda}{\mu\gamma}\right) \geq 0 \Leftrightarrow \lambda \geq \mu\gamma.$$

The other inequalities are proven analogously. $\square$

4.2 EMBEDDABILITY OF K3P MARKOV MATRICES

In this section, we adapt the results of Chapter 3 to K3P Markov matrices. Since all K3P Markov matrices diagonalize with real eigenvalues, we only consider cases I, III and IV in Lemma 3.1.1.

4.2.1 Case I: Generic K3P Matrices

The subset of Markov matrices with different eigenvalues $1, \lambda, \mu, \gamma$ is a dense subset of K3P matrices. Recall that the embeddability of such a matrix is determined by its principal logarithm (see Corollary 1.3.8 and Lemma 3.1.2). Moreover, Lemma 4.1.3 characterizes when the principal logarithm of a K3P matrix is a rate matrix. As a consequence of these results we determine the embeddability of most K3P matrices.

Corollary 4.2.1. *Let M be a K3P Markov matrix with eigenvalues $1, \lambda, \mu, \gamma$ such that λ, μ, γ are pairwise different. Then, M is embeddable if and only if the eigenvalues of M are strictly positive, and satisfy*

$$\lambda \geq \mu\gamma, \qquad \mu \geq \lambda\gamma, \qquad \gamma \geq \lambda\mu.$$

4.2.2 Case III: two repeated eigenvalues

We start by showing that the study of embeddability for K3P matrix with two repeated eigenvalues can be restricted to K2P matrices.

Lemma 4.2.2. *Let $M = K(a, b, c, d)$ be a K3P matrix with a an eigenvalue with multiplicity 2. Then there exist a 4×4 permutation matrix P such that $P^t\ M\ P$ is a K2P matrix. Moreover, Q is a Markov generator of M if and only if $P^t\ Q\ P$ is a Markov generator of $P\ M\ P$. In particular M is embeddable if and only if $P^t\ M\ P$ is embeddable*

Proof. Since M is a Markov matrix its eigenvalues are $1, \lambda, \mu, \gamma$, where λ, γ, μ are defined in (4.2). We first show that it is not possible that the only eigenvalue with multiplicity 2 of a K3P matrix is the eigenvalue 1. Indeed, if $\lambda = 1$, we derive from (4.2) that $c = d = 0$ and hence $\mu = \gamma = a - b$. Similarly, $\gamma = 1$ implies $\lambda = \mu$ an $\mu = 1$ implies $\lambda = \gamma$. Note that (4.2) yields $\mu - \gamma = c - d$, thus $\mu = \gamma$ if and only if $c = d$. Analogously, we have $\lambda = \gamma$ if and only if $b = d$ and $\lambda = \mu$ if and only if $b = c$. Therefore, if M has a two equal eigenvalues it has one of the following forms: $K(a, b, c, c)$, $K(a, b, c, b)$ or $K(a, b, b, d)$. Note that these three matrices produce a K2P by ordering the nucleotides as $(\mathtt{A}, \mathtt{G}, \mathtt{C}, \mathtt{T})$, $(\mathtt{A}, \mathtt{C}, \mathtt{G}, \mathtt{T})$ and $(\mathtt{A}, \mathtt{C}, \mathtt{T}, \mathtt{G})$ respectively (see Figure 1.1). To conclude the proof we note that reordering the nucleotides is equivalent to permute the rows and columns of M accordingly (see Section 1.4.1). $\square$

According to Theorem 3.1.10 all real logarithms with rows summing to zero of a K2P Markov matrix M with eigenvalues $1, \lambda, \mu, \mu,\ \lambda \neq \mu$ are of the form:

$$L_k(x,y,z) = L + (2\pi k + \operatorname{Arg}\mu)\, V(x,y,z), \tag{4.4}$$

where $k \in \mathbb{Z}$,

$$L = S \operatorname{diag}(0, \log(\lambda), \log|\mu|, \log|\mu|)\ S^{-1} \text{ and}$$
$$V(x,y,z) := S \operatorname{diag}\left(0, 0, \begin{pmatrix} -y & x \\ -z & y \end{pmatrix}\right)\ S^{-1}$$

for some $(x,y,z) \in \mathcal{V}_+ = \{(x,y,z) \in \mathbb{R}^3 | xz - y^2 = 1,\ x, z > 0\}$.

Note that $\operatorname{Arg}\mu$ is either 0 or π because $\mu \in \mathbb{R}$. Moreover, if $\mu > 0$, then L is the principal logarithm of M and hence $L_0(x,y,z) = \operatorname{Log}(M)$ for all $(x,y,z) \in \mathcal{V}_+$.

Lemma 4.2.3. *Let M be a K2P Markov matrix with eigenvalues $1, \lambda, \mu, \mu$, $\lambda \neq \mu$. Then, $L_k(x,y,z)$ is a Markov generator of M if and only if the following inequalities hold:*

$$\log(\lambda) - 2\log|\mu| \geq \left|2\pi k + \operatorname{Arg}\mu\right| |x - z| \tag{4.5}$$

and

$$-\log(\lambda) \geq \left|2\pi k + \operatorname{Arg}\mu\right| \left(x + z + 2|y|\right). \tag{4.6}$$

Proof. From Theorem 3.1.10 we have that $L_k(x,y,z)$ is a real logarithm of M with rows summing to 0 for all values of $k \in \mathbb{Z}$. Thus we only need to characterize those $L_k(x,y,z)$ that have non-negative entries outside the diagonal. By computing L as in (4.4) we get:

$$L = \frac{1}{4}\begin{pmatrix} \log(\lambda) + 2\log(\mu) & \log(\lambda) - 2\log(\mu) & -\log(\lambda) & -\log(\lambda) \\ \log(\lambda) - 2\log(\mu) & \log(\lambda) + 2\log(\mu) & -\log(\lambda) & -\log(\lambda) \\ -\log(\lambda) & -\log(\lambda) & \log(\lambda) + 2\log(\mu) & \log(\lambda) - 2\log(\mu) \\ -\log(\lambda) & -\log(\lambda) & \log(\lambda) - 2\log(\mu) & \log(\lambda) + 2\log(\mu) \end{pmatrix}.$$

On the other hand, we obtain the following expression for $V(x,y,z)$:

$$V(x,y,z) = \frac{1}{4}\begin{pmatrix} x-z & -x+z & -x-z-2y & x+z+2y \\ -x+z & x-z & x+z+2y & -x-z-2y \\ x+z-2y & -x-z+2y & -x+z & x-z \\ -x-z+2y & x+z-2y & x-z & -x+z \end{pmatrix}.$$

By looking at the off-diagonal entries of $L_k(x,y,z)$ (see (4.4)), we get that $L_k(x,y,z)$ is a rate matrix if and only if:

$$\begin{aligned} -\lambda + 2\mu \pm \big(2\pi k + \operatorname{Arg}\mu\big)(x-z) \geq 0 \; &(\text{entries } (1,2),(2,1),(3,4),(4,3) \geq 0) \\ \lambda \pm \big(2\pi k + \operatorname{Arg}\mu\big)(x+z+2y) \geq 0 \; &(\text{entries } (1,3),(1,4),(2,3),(2,4) \geq 0) \\ \lambda \pm \big(2\pi k + \operatorname{Arg}\mu\big)(x+z-2y) \geq 0 \; &(\text{entries } (3,1),(3,2),(4,1),(4,2) \geq 0). \end{aligned}$$

The first inequality above gives (4.5), while (4.6) follows by joining the second and third inequalities due to the fact that $\max\big(|x+z-2y|, |x+z+2y|\big) = x+y+2|y|$ as $x,z>0$. □

Below, we prove that if M is embeddable then $L_0(1,0,1)$ is necessarily a Markov generator.

Theorem 4.2.4. *Let M be a nonsingular K2P Markov matrix with eigenvalues 1, λ, μ, μ satisfying $\lambda > 0$ and $\mu \neq \lambda$. If $L_k(x,y,z)$ is a Markov generator of M for some $k \in \mathbb{Z}$, $(x,y,z) \in \mathcal{V}_+$, then we have:*

i) $L_l(x,y,z)$ is a rate matrix for any integer $l \in I_k$ where

$$I_k = \begin{cases} \langle -k, k\rangle & \text{if } \mu > 0 \\ \langle -k-1, k\rangle & \text{if } \mu < 0 \end{cases}$$

(we use the notation $\langle a, b\rangle$ to denote the closed *interval delimited by a and b, no matters if $a > b$ or $a < b$).*

ii) $L_k(1,0,1)$ is a rate matrix.

Proof. We shall prove that $L_l(x,y,z)$ and $L_0(1,0,1)$ are Markov matrices by checking that they satisfy the inequalities (4.5) and (4.6) in Lemma 4.2.3.

i) We have $|2\pi l+\operatorname{Arg}\mu| \leq |2\pi k+\operatorname{Arg}\mu|$ for any $l \in I_k$. Therefore, since the inequalities (4.5) and (4.6) are satisfied for $L_k(x,y,z)$, we deduce that they are also satisfied for $L_l(x,y,z)$.

ii) For any $(x,z,y) \in \mathcal{V}_+$ we have $xz \geq 1$ and $x+z+2|y| = x+z+2\sqrt{xz-1}$. Moreover, since $z > 0$ we obtain $z \geq 1/x$ and hence $x+z+2|y| \geq x+1/x$. Now, let us consider the real function $f(x) = \frac{1+x^2}{x}$ restricted to $\mathbb{R}_{>0}$. With this restriction on the domain of f, we can compute its derivatives $f'(x) = (x^2-1)/x^2$ and $f''(x) = 2/x^3$ for any $x \in \mathbb{R}_{>0}$. Note that $f'(x)$ only vanishes at $x = 1$ and $f''(2) = 2$, thus $f(x)$ has an absolute minimum at $x = 1$. This proves that $x+z+2|y| \geq f(1) = 2$ for any $(x,y,z) \in \mathcal{V}_+$. Moreover, in this case, $x+z+2|y| = 2$ if and only if $(x,y,z) = (1,0,1)$. Furthermore, using that $L_k(x,y,z)$ is a rate matrix and applying Lemma 4.2.3 we get:

$$\log(\lambda) - 2\log|\mu| \geq \left|2\pi k + \operatorname{Arg}\mu\right||x-z| \geq \left|2\pi k + \operatorname{Arg}\mu\right||1-1| = 0$$

and

$$-\log(\lambda) \geq \left|2\pi k + \operatorname{Arg}\mu\right|\big(x+z+2|y|\big) \geq \left|2\pi k + \operatorname{Arg}\mu\right|\big(1+1+0\big).$$

Therefore, $L_k(1,0,1)$ satisfy the inequalities (4.5) and (4.6). □

Now, we are ready to prove one of the main results in this section, which characterizes embeddable K2P Markov matrices.

Corollary 4.2.5. *Let M be a K2P matrix with eigenvalues 1, λ, μ, μ such that $\lambda \neq \mu$. Then, M is embeddable if and only if*

$$L_0(1,0,1) = S\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \log(\lambda) & 0 & 0 \\ 0 & 0 & \log|\mu| & -\operatorname{Arg}\mu \\ 0 & 0 & \operatorname{Arg}\mu & \log|\mu| \end{pmatrix} S^{-1}$$

is a rate matrix. In particular, if $\mu > 0$, then M is embeddable if and only if $\operatorname{Log}(M)$ *is a rate matrix.*

Proof. If $\lambda < 0$ or M is singular, then M is not embeddable because it has no real logarithm (see Proposition 1.3.6). For $\lambda > 0$, the first claim is a direct consequence of Theorems 3.1.10 and 4.2.4. To conclude the proof, note that if $\mu > 0$ then $L_0(1, 0, 1) = \mathrm{Log}(M)$ (see Remark 3.1.9). □

The following corollaries use the result above to characterize embeddable K2P Markov matrices in terms of its eigenvalues (Corollary 4.2.6) and in terms of its entries (Corollary 4.2.7).

Corollary 4.2.6. *Let M be a K2P Markov matrix with eigenvalues 1, λ, μ, μ. Then:*

i) If $\mu = 0$, M is not embeddable.

ii) If $\mu > 0$, M is embeddable if and only if $\lambda \geq \mu^2$.

iii) If $\mu < 0$, M is embeddable if and only if $e^{-2\pi} \geq \lambda \geq \mu^2$.

Proof. By Corollary 4.2.5 we know that M is embeddable if and only if $L_0(1, 0, 1)$ is a rate matrix. If $\lambda \neq \mu$, from Lemma 4.2.3 we have that $L_0(1, 0, 1)$ is a rate matrix if and only if $\log(\lambda) - 2\log|\mu| \geq 0$ and $-\log(\lambda) \geq 2\,\mathrm{Arg}\,\mu$. The claim follows by taking exponentials and rearranging the terms in these inequalities. For $\lambda = \mu$, M is a JC matrix which is known to be embeddable if and only if its eigenvalues are positive (see Proposition 3.1.14). Note that if $\lambda = \mu$, the inequality $\lambda \geq \mu^2$ is satisfied if and only if $\lambda \in [0, 1]$. By Proposition 1.2.5 i) we have that $\lambda \leq 1$, thus the statement also holds if $\lambda = \mu$. □

Corollary 4.2.7. *Let $M = K(1 - b - 2c, b, c, c)$ be a K2P Markov matrix. Then:*

i) If $c = 0.5 - b$, M is not embeddable.

ii) If $c < 0.5 - b$, M is embeddable if and only if $c \leq \sqrt{b} - b$.

iii) If $c > 0.5 - b$, M is embeddable if and only if $\frac{1-e^{-2\pi}}{4} \leq c \leq \sqrt{b} - b$.

Proof. The claim follows from Corollary 4.2.6 by expressing the eigenvalues in terms of the entries. In this case, we have $\lambda = 1 - 4c$, $\mu = 1 - 2b - 2c$ (see (4.2)). It is clear that the cases in both results are the same. Now, $\lambda \leq \mu^2$ is equivalent to $0 \leq (\mu^2 - \lambda)/4 = c^2 + 2bc + b^2 - b$. This inequality is satisfied if and only if $c \in [-b - \sqrt{b}, -b + \sqrt{b}]$. Since M is a Markov matrix we have that $c > 0$ and also that $b \in [0, 1]$. Therefore, $\lambda \leq \mu^2$ is equivalent to $0 < c < \sqrt{b} - b$. Finally, it is immediate to check that $e^{-2\pi} \geq \lambda$ is equivalent to $\frac{1}{4} - \frac{e^{-2\pi}}{4} \leq c$. □

Remark 4.2.8. The third item in Corollary 4.2.6 (or in Corollary 4.2.7) shows that there are embeddable K3P matrices with negative eigenvalues. These matrices are embeddable but are not model-embeddable because their principal logarithm is not a real matrix (see Theorem 4.1.2). This fact exhibits that the structure of the K3P model, which imposes certain symmetries between transitions and between transversions, is not always captured by the same symmetries between the mutation rates (cf. [Kim80, Kim81]). Moreover, this also shows that embeddability is not necessarily determined by the principal logarithm (cf. [VYP+13, AKK21]).

4.2.3 Case IV: JC Matrices

If a K3P matrix has three repeated eigenvalues, then it is a JC matrix. Therefore, all JC Markov matrix with positive determinant are embeddable by Proposition 3.1.14. In this case, its principal logarithm is a rate matrix and it is a JC matrix too (see Theorem 4.1.2).

4.3 IDENTIFIABILITY OF RATES FOR K2P MARKOV MATRICES

We know that generic K3P embeddable matrices have different eigenvalues and hence they have identifiable rates by Corollary 1.3.8. In this section we address the rate identifiability problem for K2P embeddable matrices. Actually, by Lemma 4.2.2, the results in this section can be applied to any K3P matrix with an eigenvalue with multiplicity 2, regardless of whether they are K2P matrices or not.

As a consequence of the results obtained in previous section, we provide a criterion to determine whether the rates of K2P embeddable matrices are identifiable or not. Furthermore, for those matrices with non-identifiable rates we determine how many Markov generators they admit.

Proposition 4.3.1. *Let M be an embeddable K2P Markov matrix with eigenvalues 1, λ, μ, μ with $\lambda \neq \mu$. Then, the rates of M are identifiable if and only if $L_{-1}(1,0,1)$ is not a rate matrix.*

Proof. By Corollary 4.2.5 we know that M is embeddable if and only if $L_0(1,0,1)$ is a rate matrix. Now, assume that there are $(x,y,z) \in \mathcal{V}_+$ and $k \in \mathbb{Z}$ such that $L_k(x,y,z)$ is a Markov generator of M different than $L_0(1,0,1)$. This implies that $k \neq 0$ if $\mu > 0$ (see Remark 3.1.9). Hence, Theorem 4.2.4 gives that $L_{-1}(1,0,1)$ is also Markov generator because -1 belongs to the interval I_k, independently of the sign of μ. Note that $L_0(1,0,1)$ and $L_{-1}(1,0,1)$ are distinct Markov generators by Theorem 3.1.10. □

Example 4.3.2. Here we show an embeddable K2P Markov matrix with negative eigenvalues and non-identifiable rates. Take M as K2P Markov matrix with eigenvalues 1, $\lambda = e^{-2\pi}$ and $\mu = -e^{-\pi}$ (with multiplicity 2). Rounding to the 10th decimal the entries of M are:

$$M = \begin{pmatrix} 0.2288599016 & 0.2720738198 & 0.2495331393 & 0.2495331393 \\ 0.2720738198 & 0.2288599016 & 0.2495331393 & 0.2495331393 \\ 0.2495331393 & 0.2495331393 & 0.2288599016 & 0.2720738198 \\ 0.2495331393 & 0.2495331393 & 0.2720738198 & 0.2288599016 \end{pmatrix}.$$

As we can see, $\mathrm{Log}(M)$ is not a real matrix:

$$\mathrm{Log}(M) = \frac{1}{2} \begin{pmatrix} -2\pi + \pi\, i & -\pi\, i & \pi & \pi \\ 3\pi - \pi\, i & -2\pi + \pi\, i & \pi & \pi \\ \pi & \pi & -2\pi + \pi\, i & -\pi\, i \\ \pi & \pi & -\pi\, i & -2\pi + \pi\, i \end{pmatrix}.$$

In spite of that, $L_0(1,0,1)$ is a rate matrix, so M is embeddable. Furthermore, $L_{-1}(1,0,1)$ is also a Markov generator of M and hence the rates are not identifiable. Indeed,

$$L_0(1,0,1) = \begin{pmatrix} -\pi & 0 & 0 & \pi \\ 0 & -\pi & \pi & 0 \\ \pi & 0 & -\pi & 0 \\ 0 & \pi & 0 & -\pi \end{pmatrix}$$

and

$$L_{-1}(1,0,1) = \begin{pmatrix} -\pi & 0 & \pi & 0 \\ 0 & -\pi & 0 & \pi \\ \pi & 0 & -\pi & 0 \\ 0 & \pi & 0 & -\pi \end{pmatrix}.$$

Remark 4.3.3. We derive easily that the product of embeddable matrices within the Kimura 2ST model is not necessarily embeddable (cf. Lemma 4.1.1). Indeed, it is enough to consider the embeddable matrix M in the previous example and any K3P matrix N with positive eigenvalues $1, \lambda, \mu, \gamma$ satisfying the inequalities (4.3) so that N is embeddable. The product of M and N is clearly a K3P Markov matrix, whose eigenvalues are the product of the eigenvalues of M and N. Thus, MN has two *different negative* eigenvalues and another positive eigenvalue. According to Proposition 1.3.6, MN has no real logarithm so, in particular, it cannot be embeddable.

Example 4.3.4. In this example we show an embeddable K2P Markov matrix with positive eigenvalues and non-identifiable rates. Let us consider M the K2P Markov matrix with eigenvalues 1, $\lambda = e^{-4\pi}$ and $\mu = e^{-2\pi}$ (with multiplicity 2). Rounding to the 10th decimal the entries of M are:

$$M = \begin{pmatrix} 0.2509345932 & 0.2490671504 & 0.2499991282 & 0.2499991282 \\ 0.2490671504 & 0.2509345932 & 0.2499991282 & 0.2499991282 \\ 0.2499991282 & 0.2499991282 & 0.2509345932 & 0.2490671504 \\ 0.2499991282 & 0.2499991282 & 0.2490671504 & 0.2509345932 \end{pmatrix}.$$

We have that $\mathrm{Log}(M)$ is a Markov generator and hence M is embeddable. Indeed,

$$\mathrm{Log}(M) = \begin{pmatrix} -2\pi & 0 & \pi & \pi \\ 0 & -2\pi & \pi & \pi \\ \pi & \pi & -2\pi & 0 \\ \pi & \pi & 0 & -2\pi \end{pmatrix}.$$

Nonetheless, the rates of M are not identifiable because there are other Markov generators for it:

$$L_{-1}(1,0,1) = \begin{pmatrix} -2\pi & 0 & 2\pi & 0 \\ 0 & -2\pi & 0 & 2\pi \\ 0 & 2\pi & -2\pi & 0 \\ 2\pi & 0 & 0 & -2\pi \end{pmatrix},$$

and

$$L_{1}(1,0,1) = \begin{pmatrix} -2\pi & 0 & 0 & 2\pi \\ 0 & -2\pi & 2\pi & 0 \\ 2\pi & 0 & -2\pi & 0 \\ 0 & 2\pi & 0 & -2\pi \end{pmatrix}.$$

Remark 4.3.5. In Examples 4.3.2 and 4.3.4, the Markov generators other than the principal logarithm are not K3P matrices, they belong to one of the Lie Markov models listed in [FSSJW15], namely the model 3.3b. This is another 3-dimensional model, different from the K3P model, which contains the K2P model as well.

Theorem 4.3.6. *Let M be an embeddable K2P Markov matrix with eigenvalues 1, λ, μ, μ with $\lambda \neq \mu$. The following holds:*

i) If $\mu > 0$ and $\lambda > e^{-4\pi}$, then M has only one Markov generator, which is its principal logarithm.

ii) If $\mu > 0$ and $\lambda = e^{-4\pi}$, then M has exactly 3 generators: $\mathrm{Log}(M)$, $L_1(1,0,1)$ and $L_{-1}(1,0,1)$.

iii) If $\mu < 0$ and $\lambda = e^{-2\pi}$ then M has exactly 2 generators: $L_0(1,0,1)$ and $L_{-1}(1,0,1)$.

In any other case, M has uncountable Markov generators.

Proof. Since M is embeddable we have that $\lambda \geq \mu^2$ (see Corollary 4.2.6). Let us also recall that for any $(x,y,z) \in \mathcal{V}_+$ we have $x+z+2|y| \geq 2$ and the equality is obtained only for $(x,y,z) = (1,0,1)$ (see the proof of Theorem 4.2.4).

i) We know that $L_{-1}(1,0,1)$ is not a rate matrix by Lemma 4.2.3. Hence, by Proposition 4.3.1 the rates of M are identifiable. Furthermore, due to Corollary 4.2.5 we have that the only Markov generator of M must be its principal logarithm.

ii) Let $L_k(x,y,z)$ be a Markov generator of M with $(x,y,z) \in \mathcal{V}_+$. From inequality (4.6) in Lemma 4.2.3 we have that $4\pi \geq 2|k|\pi\ (x+z+2|y|)$. Using that $(x+z+2|y|) > 2$ for $(x,y,z) \neq (1,0,1)$ we get that the inequality holds if and only if $k=0$ (and hence $L_0(x,y,z) = \mathrm{Log}(M)$) or $(x,y,z) = (1,0,1)$ and $|k| = 1$.

iii) Let $Q := L_k(x,y,z)$ be a Markov generator of M with $(x,y,z) \in \mathcal{V}_+$. It follows from inequality (4.6) in Lemma 4.2.3 that $2\pi \geq \big|2k+1|\pi\ (x+z+2|y|)\big|$. Using again that $(x+z+2|y|) > 2$ for $(x,y,z) \neq (1,0,1)$ we derive that the inequality holds if and only if $(x,y,z) = (1,0,1)$ and $|2k+1| \leq 1$.

Given $(x,y,z) \in \mathcal{V}_+$ with $x = z$, we have that $L_{-1}(x,y,z)$ satisfies inequality (4.5) in Lemma 4.2.3. If $\mu > 0$ and $\lambda < e^{-4\pi}$ then inequality (4.6) is satisfied for $L_{-1}(1,0,1)$. Furthermore, inequality (4.6) is satisfied for $L_{-1}(x,y,x)$ provided that $(x,y,x) \in \mathcal{V}_+$ is close enough to $(1,0,1)$. Hence, Lemma 4.2.3 implies that $L_{-1}(x,y,z)$ is a Markov generator of M for any $(x,y,z) \in \mathcal{V}_+$ close enough to $(1,0,1)$ satisfying $x = z$. The same argument does also work for $\mu < 0$ and $\lambda < e^{-2\pi}$. □

Remark 4.3.7. Theorem 4.3.6 proves that the matrices in Examples 4.3.2 and 4.3.4 do not admit any Markov generator other than the shown there. Moreover, embeddable matrices with non-identifiable rates must satisfy $\lambda \geq \mu^2$, hence they have determinant $\leq e^{-8\pi}$ if all the eigenvalues are positive, and determinant $\leq e^{-4\pi}$ if they have a repeated negative eigenvalue. In particular, the matrices in these examples are precisely the K2P embeddable matrices with no-identifiable rates with greater determinant for each case (negative and positive eigenvalues respectively). This implies that, in the framwork of the continuous K2P model, we can guarantee identifiability of rates as long as the expected number of elapsed nucleotide substitution per site is lower than π (see Remark 1.4.9)

Figure 4.1 below illustrates Corollary 4.2.6 and Theorem 4.3.6. Note that the space of embeddable matrices with no identifiable rates has positive measure within the space of all K2 Markov matrices.

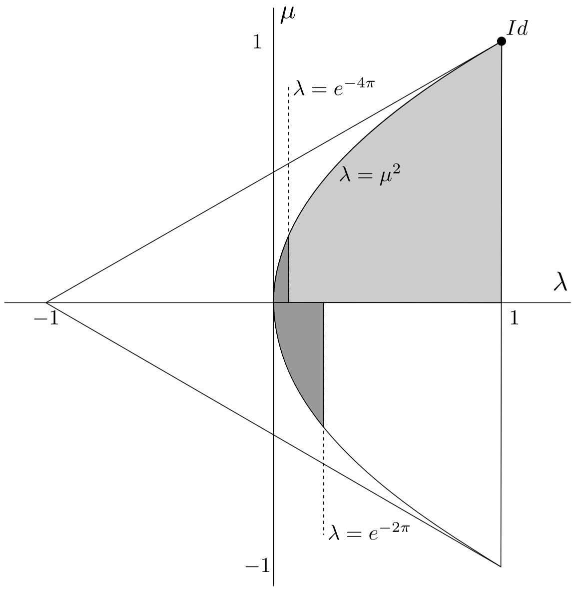

Figure 4.1: Parameterizations of K2P Markov matrices in terms of their eigenvalues λ and μ. Embeddable matrices with only one Markov generator appear in light grey and embeddable matrices with infinitely many Markov generators in dark grey. The vertical segments delimiting the dark regions contain embeddable matrices without identifiable rates but a finite number of Markov generators. The scale in this figure is not exact so that the dark grey areas could be visualized.

We can characterize rate identifiability of K2P matrices in terms of their entries rather than in terms of its eigenvalues as we did for embeddability in Corollary 4.2.7. All together, the main results in this chapter for the K2P model are summarized in the following result (see also Figure 4.2).

Theorem 4.3.8. *For any given K2P Markov matrix $M = K(a, b, c, c)$, the following holds:*

a) If $c = 0.5 - b$, then M is not embeddable.

b) If $c < 0.5 - b$, M is embeddable if and only if $c \leq \sqrt{b} - b$. In this case,

i) If $c < \frac{1-e^{-4\pi}}{4}$, then the rates of M are identifiable.

ii) If $c = \frac{1-e^{-4\pi}}{4}$, then M has exactly 3 Markov generators.

iii) If $c > \frac{1-e^{-4\pi}}{4}$, then M has infinitely many Markov generators.

c) If $c > 0.5 - b$, M is embeddable if and only if $\frac{1-e^{-2\pi}}{4} \leq c \leq \sqrt{b} - b$. In this case the rates of M are not identifiable. Moreover,

i) If $c = \frac{1-e^{-2\pi}}{4}$, then M has exactly 2 Markov generators.

ii) If $c > \frac{1-e^{-2\pi}}{4}$, then M has infinitely many Markov generators.

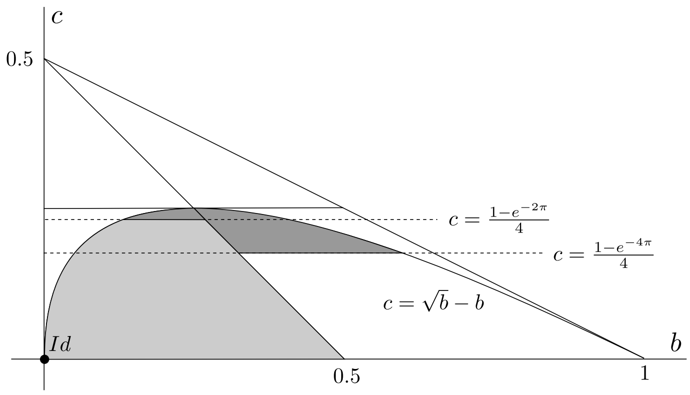

Figure 4.2: Parameterizations of K2P Markov matrices in terms of their entries b and c. Embeddable matrices with only one Markov generator appear in light grey and embeddable matrices with infinitely many Markov generators in dark grey. The horizontal segments delimiting the dark regions contain embeddable matrices without identifiable rates but a finite number of Markov generators. The scale in this figure is not exact so that the dark grey areas could be visualized.

4.4 VOLUME OF EMBEDDABLE MATRICES FOR THE K3P MODEL AND ITS SUBMODELS

The goal of this section is to take advantage of the characterization of embeddability of K3P, K2P and JC matrices in terms of the eigenvalues in order to measure how big the set of embeddable matrices is within each of these models. This can be measured in terms of the volume of the corresponding subspaces and clarifies how restrictive is to consider homogeneous continuous-time models. At the same time, we will obtain the volume of some relevant subsets of Markov matrices with some constraints to make them mathematically or biologically meaningful (see Definition 1.4.11).

Remark 4.4.1. For the K3P model, the subsets introduced in Definition 1.4.11 can be expressed in terms of its entries a, b, c, d:

- Δ^{K3P} is the set of all K3P Markov matrices, i.e. $a+b+c+d = 1$ and $a, b, c, d \geq 0$.
- $\Delta^{\text{K3P}}_{\text{dlc}}$ is the set of K3P Markov matrices with $a \geq b, c, d$.
- $\Delta^{\text{K3P}}_{\text{dd}}$ is the set of all $M \in \Delta^{\text{K3P}}$ with $a \geq b + c + d$ or equivalently $a \geq 0.5$.
- $\Delta^{\text{K3P}}_{\text{Id}}$ is the set of all $M \in \Delta^{\text{K3P}}$ with positive eigenvalues (see Remark 1.4.12). According to (4.2) this is the set of $M \in \Delta^{\text{K3P}}$ satisfying $a + b > c + d$, $a + c > b + d$ and $a + d > b + c$.
- $\Delta^{\text{K3P}}_{\text{emb}}$ is the set of all embeddable K3P Markov matrices.

By using this, it is immediate to check that $\Delta^{\text{K3P}}_{\text{dd}} \subset \Delta^{\text{K3P}}_{\text{Id}} \subset \Delta^{\text{K3P}}_{\text{dlc}} \subset \Delta^{\text{K3P}}$ (cf. Remark 1.4.12). Also note that the description of $\Delta^{\text{K3P}}_{\cdot}$ in terms of the entries of K3P matrices can be adapted to the K2P model and the JC model by imposing $c = d$ and $b = c = d$ respectively. Hence, the inclusions above are also valid for these two models.

4.4.1 The volume of embeddable K3P matrices

In order to compute the volumes of the sets introduced above, note that every K3P matrix $K(a,b,c,d)$ is a convex combination of the identity matrix and the permutation matrices

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

with coefficients $a,b,c,d \geq 0$ satisfying $a+b+c+d=1$. Moreover, Lemma 4.0.1 allows the identification of K3P Markov matrices with a 3-dimensional space by using the coordinates (λ,μ,γ). Hence, the space of all K3P Markov matrices describes the 3-dimensional simplex (a regular tetrahedron) whose vertices correspond to the permutation matrices above. The coordinates of the vertices are given by their corresponding eigenvalues: $p_1 = (1,1,1)$, $p_2 = (1,-1,-1)$, $p_3 = (-1,1,-1)$ and $p_4 = (-1,-1,1)$ (see Figure 4.3). The centroid of this simplex has coordinates (eigenvalues) $O = (0,0,0)$ and corresponds to the matrix

$$M = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

According to this representation, JC matrices ($b=c=d$) correspond to the line through p_1 and the centroid O, while K2P matrices ($c=d$) correspond to a plane section of the simplex ($\mu=\gamma$).

Proposition 4.4.2. *Consider the subsets of K3P Markov matrices in Remark 4.4.1. Then:*

i) $\frac{V(\Delta_{\mathrm{dlc}}^{\mathrm{K3P}})}{V(\Delta^{\mathrm{K3P}})} = \frac{1}{4}$, $\frac{V(\Delta_{\mathrm{Id}}^{\mathrm{K3P}})}{V(\Delta^{\mathrm{K3P}})} = \frac{3}{16}$, $\frac{V(\Delta_{\mathrm{dd}}^{\mathrm{K3P}})}{V(\Delta^{\mathrm{K3P}})} = \frac{1}{8}$ *and* $\frac{V(\Delta_{\mathrm{emb}}^{\mathrm{K3P}})}{V(\Delta^{\mathrm{K3P}})} = \frac{3}{32}$.

ii) $\frac{V(\Delta_{\mathrm{emb}}^{\mathrm{K3P}} \cap \Delta_{\mathrm{Id}}^{\mathrm{K3P}})}{V(\Delta_{\mathrm{emb}}^{\mathrm{K3P}})} = 1$, $\frac{V(\Delta_{\mathrm{emb}}^{\mathrm{K3P}} \cap \Delta_{\mathrm{dd}}^{\mathrm{K3P}})}{\Delta_{\mathrm{dd}}^{\mathrm{K3P}}} \simeq 0.61008$.

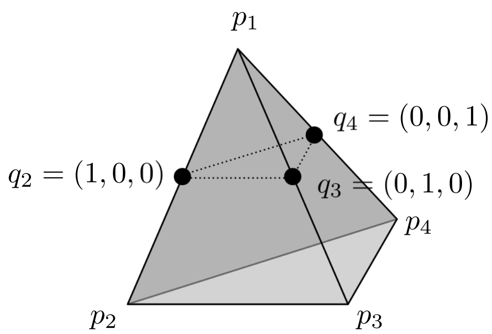

Figure 4.3: Simplex representing all K3 Markov matrices. Each matrix is represented by its eigenvalues (λ, μ, γ).

Proof. We compute the volumes of each subset in Definition 1.4.11 for the K3P model in the space of K3P Markov parametrized by its eigenvalues (λ, μ, γ). The claim follows by computing the corresponding quotients. Note that the change from the coordinates given by the entries (b, c, d) to the coordinates in terms of the eigenvalues (λ, μ, γ) is given by an affine transformation (see (4.2)) and hence it preserves the proportion of volumes. The determinant of the corresponding linear map is equal to -16. Therefore, the volume of any subset of K3P Markov matrices is sixteen times larger in the parametrization in terms of the eigenvalues. However, it is clear that the relative volumes do not depend on the parametrization. Before start computing the volumes of the sets, we recall that the volume of a tetrahedron with vertices p_1, p_2, p_3, p_4 is given by the well known formula

$$V = \frac{1}{6} \,|\det(\overrightarrow{p_1 p_2}, \overrightarrow{p_1 p_3}, \overrightarrow{p_1 p_4})|. \tag{4.7}$$

i) The space $\Delta_{\mathrm{dd}}^{\mathrm{K3P}}$ of diagonal dominant matrices is defined by the inequality $a \geq b + c + d$. Since $a + b + c + d = 1$, this is equivalent to $a \geq 1/2$. Thus, $\Delta_{\mathrm{dd}}^{\mathrm{K3P}}$ is the regular simplex with vertices p_1, q_2, q_3 and q_4 (see Figure 4.3) and $V(\Delta_{\mathrm{dd}}^{\mathrm{K3P}}) = \frac{1}{3}$ by (4.7).

The space $\Delta_{\mathrm{Id}}^{\mathrm{K3P}}$ of matrices with positive eigenvalues is composed of $\Delta_{\mathrm{dd}}^{\mathrm{K3P}}$ together with the simplex with vertices q_2, q_3, q_4 and the centroid O. The formula in (4.7) gives that this last simplex has volume 1/6. Therefore, $V(\Delta_{\text{Id}}^{\text{K3P}}) = V(\Delta_{\text{dd}}^{\text{K3P}}) + 1/6 = 1/2$.

The three inequalities defining $\Delta_{\text{dlc}}^{\text{K3P}}$ are equivalent to $\lambda + \mu \geq 0$, $\lambda + \gamma \geq 0$ and $\mu + \gamma \geq 0$ (see (4.2)). If we denote by p_{ijk} the centroid of the triangle defined by p_i, p_j and p_k, it is straighforward to see that $\Delta_{\text{dlc}}^{\text{K3P}}$ is formed by $\Delta_{\text{Id}}^{\text{K3P}}$ together with the three simplices defined by $\{O, q_2, q_3, p_{123}\}$, $\{O, q_3, q_4, p_{134}\}$ and $\{O, q_4, q_2, p_{124}\}$. According to (4.7), the volume of these three simplices is 1/18. Therefore, $V(\Delta_{\text{dlc}}^{\text{K3P}}) = 1/2 + 3\,(1/18) = 2/3$.

Δ^{K3P} is the tetrahedron with vertices $p_1 = (1,1,1)$, $p_2 = (1,-1,-1)$, $p_3 = (-1,1,-1)$ and $p_4 = (-1,-1,1)$ (see Figure 4.3). In this case, (4.7) yields $V(\Delta^{\text{K3P}}) = 8/3$.

Before computing $V(\Delta_{\text{emb}}^{\text{K3P}})$, note that all embeddable K3P matrices with a negative eigenvalue have a repeated eigenvalue (see Section 4.2). Therefore, they are a marginal case with measure (i.e. volume) zero within the whole set of K3P Markov matrices. Hence, the volume of the space $\Delta_{\text{emb}}^{\text{K3P}}$ can be computed using the conditions in Corollary 4.2.1. This implies that $\lambda, \gamma, \mu > 0$. Moreover, the range of values for μ is between $\gamma\,\lambda$ and λ/γ if $\lambda \leq \gamma$. Conversely, μ lies between $\gamma\,\lambda$ and γ/λ if $\gamma \leq \lambda$. Hence, we are led to compute the following integral

$$V(\Delta_{\text{emb}}^{\text{K3P}}) = \int_0^1 \left(\int_0^{\gamma} \int_{\gamma\lambda}^{\lambda/\gamma} d\mu\, d\lambda + \int_{\gamma}^{1} \int_{\lambda\gamma}^{\gamma/\lambda} d\mu\, d\lambda \right) d\gamma$$

which can be easily shown to be equal to 1/4.

ii) As noted above, the set of embeddable matrices that are not in $\Delta_{\text{Id}}^{\text{K3P}}$ has measure (i.e. volume) zero within Δ^{K3P}. Therefore, we have $V(\Delta_{\text{emb}}^{\text{K3P}} \cap \Delta_{\text{Id}}^{\text{K3P}}) = V(\Delta_{\text{emb}}^{\text{K3P}})$.

On the other hand, the Markov matrix in Example 4.3.2 is embeddable but not DLC, thus $\Delta_{\text{emb}}^{\text{K3P}} \not\subset \Delta_{\text{dlc}}^{\text{K3P}}$. The computation of the volume of the intersection $\Delta_{\text{dd}}^{\text{K3P}} \cap \Delta_{\text{emb}}^{\text{K3P}}$ is similar to the computation of $V(\Delta_{\text{emb}}^{\text{K3P}})$ but for each value of $\gamma \in [0,1]$ we have to remove the area of the space below the line $\lambda + \mu = 1 - a$ (corresponding to non-embeddable matrices). This leads to two different situations: for $\gamma \in [0, 3 - 2\sqrt{2}]$ the line cuts the hyperbola $\lambda\mu = \gamma$; whereas for $\gamma \in [3 - 2\sqrt{2}, 1]$ the line and the hyperbola do not meet. The computation of the corresponding integrals has been obtained using the mathematical software SAGE [S+12]. □

From the previous theorem and the fact that $\Delta_{dd}^{K3P} \subset \Delta_{Id}^{K3P} \subset \Delta_{dlc}^{K3P} \subset \Delta$ (see Remark 4.4.1), we can compute the relative volumes of embeddable matrices in each of the above subsets of K3P Markov matrices. This is shown in Table 4.1. These relative volumes are a measure of how many matrices are rejected when taking the homogeneoues continuous-time approach.

	Δ^{K3P}	Δ_{dlc}^{K3P}	Δ_{Id}^{K3P}	Δ_{dd}^{K3P}	Δ_{emb}^{K3P}
$\frac{V(\cdot)}{V(\Delta^{K3P})}$	1	1/4	3/16	1/8	3/32
$\frac{V(\Delta_{emb}^{K3P} \cap \cdot)}{V(\cdot)}$	3/32	3/8	1/2	0.61008	1

Table 4.1: Relative volumes of relevant subsets of K3P Markov matrices and proportion of embeddable matrices within each of them.

Remark 4.4.3. Theorem 4.1.2 implies that all the values of Table 4.1 remain the same if we only consider $K3P$-embeddable matrices (instead of embeddable matrices). This is due to the fact that the set of K3P Markov matrices with a repeated eigenvalue has measure zero within Δ^{K3P} together with Corollary 1.3.8.

4.4.2 The volume of embeddable K2P matrices

In the previous sections we have been using two different parameterizations for the set of K2P Markov matrices (see Figures 4.1 and 4.2), one in terms of the eigenvalues of the Markov matrix (λ and μ) and the other in terms of its entries (b and c). The first parametrization can be used to describe Δ_{Id}^{K2P}, whereas the second provides an easier description of Δ_{dlc}^{K2P} and Δ_{dd}^{K2P}. Figures 4.4 and 4.5 illustrate these sets and the inclusions between them (see Remark 4.4.1) in terms of the eigenvalues and the entries of the Markov matrix, respectively. For a clearer picture of embeddability and rate identifiability within each of these subsets of K2P Markov matrices, intersect Figures 4.1 and 4.4 or Figures 4.2 and 4.5.

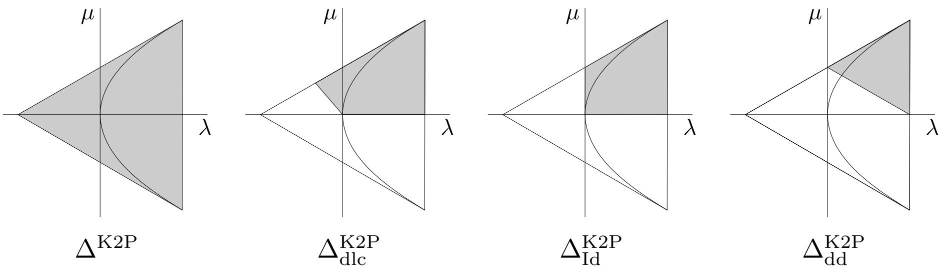

Figure 4.4: Relevant subsets of K2P Markov matrices parametrized in terms of the eigenvalues λ and μ (in grey).

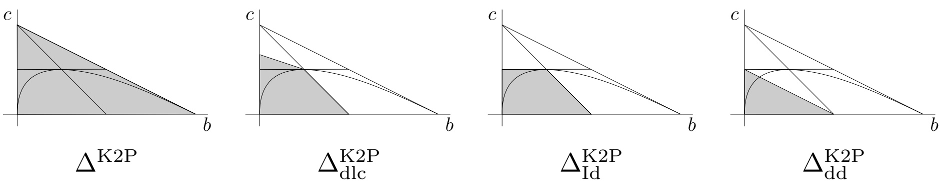

Figure 4.5: Relevant subsets of K2P Markov matrices parametrized in terms of the entries b and c (in grey).

Proposition 4.4.4. *Consider the subsets of K2P Markov matrices in Remark 4.4.1 and let* $\Delta^{\mathrm{K2P}}_{\mathrm{idf}} \subset \Delta^{\mathrm{K2P}}_{\mathrm{emb}}$ *be the subset of embeddable K2P matrices with identifiable rates. Let* α *denote the area of the space of all K2P Markov matrices,* Δ^{K2P}*. Then:*

i) $V(\Delta^{\mathrm{K2P}}_{\mathrm{dlc}}) = \frac{5\alpha}{12}$, $V(\Delta^{\mathrm{K2P}}_{\mathrm{Id}}) = \frac{3\alpha}{8}$, $V(\Delta^{\mathrm{K2P}}_{\mathrm{dd}}) = \frac{\alpha}{4}$, $V(\Delta^{\mathrm{K2P}}_{\mathrm{emb}}) = \frac{(1+e^{-3\pi})\alpha}{3}$ *and* $V(\Delta^{\mathrm{K2P}}_{\mathrm{idf}}) = \frac{(1-e^{-6\pi})\alpha}{3}$.

ii) $\Delta^{\mathrm{K2P}}_{\mathrm{emb}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{dlc}} = \Delta^{\mathrm{K2P}}_{\mathrm{emb}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{Id}}$. *Moreover,* $V(\Delta^{\mathrm{K2P}}_{\mathrm{emb}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{Id}}) = \frac{\alpha}{3}$.

iii) $\Delta^{\mathrm{K2P}}_{\mathrm{dd}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{emb}} = \Delta^{\mathrm{K2P}}_{\mathrm{dd}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{idf}}$. *Moreover,* $V(\Delta^{\mathrm{K2P}}_{\mathrm{emb}} \cap \Delta^{\mathrm{K2P}}_{\mathrm{dd}}) = \frac{(7-4\sqrt{2})\alpha}{3}$.

Proof. We compute the areas of each subset in Definition 1.4.11 for the K2P model in the 2-dimensional space parametrized by its eigenvalues (λ, μ). The claim follows by computing the corresponding quotients.
Note that the change from the coordinates given by the entries (b, c) to the coordinates in terms of the eigenvalues (λ, μ) is given by the affine transformation

$$\begin{array}{rccc} \varphi: & \text{Entries} & \longrightarrow & \text{Eigenvalues} \\ & (b,c) & \longmapsto & (1-4c\ ,\ 1-2b-2c) \end{array}$$

and hence it preserves the proportion of volumes. The determinant of the corresponding linear map is equal to -8. Therefore, the volume of any subset of K2P Markov matrices is eight times larger in the parametrization in terms of the eigenvalues. However, it is clear that the relative volumes do not depend on the parametrization. We shall use the parametrization in terms of the eigenvalues to compute the volumes because the expressions involved are simpler. In this context, we have that Δ^{K2P} is the triangle with vertices $(-1,0)$, $(1,1)$ and $(1,-1)$ which has area 2, so $\alpha = 2$.

i) $\Delta_{\text{dlc}}^{\text{K2P}}$ is the polygon with vertices $(-1/3, 1/3)$, $(1,1)$, $(1,0)$ and $(0,0)$ which has area $10/12$.

$\Delta_{\text{Id}}^{\text{K2P}}$ is the trapezoid with vertices $(0,1/2)$, $(1,1)$, $(1,0)$ and $(0,0)$ which has area $3/4$.

$\Delta_{\text{dd}}^{\text{K2P}}$ is the triangle with vertices $(0,1/2)$, $(1,1)$ and $(1,0)$ which has area $1/2$.

According to Corollary 4.2.6 we have $V(\Delta_{\text{emb}}^{\text{K2P}}) = \int_0^1 \int_{\mu^2}^1 1\ d\lambda d\mu\ + \int_{-e^{-\pi}}^0 \int_{\mu^2}^{e^{-2\pi}} 1\ d\lambda d\mu = \dfrac{2(1+e^{-3\pi})}{3}$.

According to Theorem 4.3.6, we have that $V(\Delta_{\text{idf}}^{\text{K2P}}) = \int_0^1 \int_{\mu^2}^1 1\ d\lambda d\mu - \int_0^{e^{-2\pi}} \int_{\mu^2}^{e^{-4\pi}} 1\ d\lambda d\mu = \dfrac{2(1-e^{-6\pi})}{3}$.

ii) If $M \in \left(\Delta^{\text{K2P}}_{\text{emb}} \cap \Delta^{\text{K2P}}_{\text{dlc}}\right)^C$ then its eigenvalue λ is negative, so $\lambda \ngeq \mu^2$ and M is not embeddable, which proves that $\Delta^{\text{K2P}}_{\text{emb}} \cap \Delta^{\text{K2P}}_{\text{dlc}} = \Delta^{\text{K2P}}_{\text{emb}} \cap \Delta^{\text{K2P}}_{\text{Id}}$ (see Figure 4.4). It follows from Corollary 4.2.6 that the volume of this set can be computed as $\displaystyle\int_0^1 \sqrt{\lambda}\; d\lambda = 2/3$.

iii) The set of diagonally-dominant matrices is the triangle with vertices $(0, 0.5)$, $(1, 1)$ and $(1, 0)$. According to Theorem 1.3.10 i), diagonally-dominant Markov matrices have only one real logarithm and hence the first equality follows. Furthermore the points where the curve $\mu^2 = \lambda$ intersects with the boundary of $\Delta^{\text{K2P}}_{\text{dd}}$ are $(3 - 2\sqrt{2}, -1 + \sqrt{2})$ and $(1, 1)$, thus it follows from Corollary 4.2.6 that the volume can be computed as $\displaystyle\int_{\sqrt{2}-1}^1 \int_{\mu^2}^1 1\; d\lambda d\mu + 2(\sqrt{2} - 1)^2 = \frac{7 - 4\sqrt{2}}{3}$. □

	$\frac{V(\cdot)}{V(\Delta^{\text{K2P}})}$	$\frac{V(\Delta^{\text{K2P}}_{\text{emb}} \cap\, \cdot)}{V(\cdot)}$	$\frac{V(\Delta^{\text{K2P}}_{\text{idf}} \cap\, \cdot)}{V(\Delta^{\text{K2P}}_{\text{emb}} \cap\, \cdot)}$
Δ^{K2P}	1	$\frac{1+e^{-3\pi}}{3} \approx 0.33336$	$\frac{1-e^{-6\pi}}{1+e^{-3\pi}} \approx 0.99992$
$\Delta^{\text{K2P}}_{\text{dlc}}$	$0.41\widehat{6}$	0.8	$1 - e^{-6\pi} \approx 1.00000$
$\Delta^{\text{K2P}}_{\text{Id}}$	0.375	$0.\widehat{8}$	$1 - e^{-6\pi} \approx 1.00000$
$\Delta^{\text{K2P}}_{\text{dd}}$	0.25	$\frac{14-8\sqrt{2}}{3} \approx 0.89543$	1

Table 4.2: The first column shows the relative volumes of relevant spaces in the K2P model, the second column displays the relative volumes of embeddable matrices within those spaces and the third column contains the relative volume of embeddable matrices with identifiable rates within the subset of embeddable matrices for each of the spaces. The values are rounded to the 5th decimal.

Table 4.2 shows the relative volumes of the regions defined at the beginning of this section as well as the proportion of embeddable matrices within them. The values are obtained from the preceding proposition together with the inclusions in Remark 4.4.1 (see Figures 4.4 and 4.5).

Remark 4.4.5. Recall that all embeddable K3P matrices with positive eigenvalues are also model embeddable (see Theorem 4.1.2). Hence, by Proposition 4.4.4 ii) we have that the relative volumes of K2P-embeddable matrices within Δ^{K2P} is equal to 1/3. Moreover, within $\Delta^{\mathrm{K2P}}_{\mathrm{dlc}}$, $\Delta^{\mathrm{K2P}}_{\mathrm{Id}}$ and $\Delta^{\mathrm{K2P}}_{\mathrm{dd}}$, all embeddable matrices are model-embeddable.

4.4.3 The volume of embeddable JC matrices

The computation of the sets introduced in Definition 1.4.11 for the JC model can be easily inferred from Remark 4.4.1 and Proposition 3.1.14. Indeed, for the JC model we have

$$\begin{aligned}
\Delta^{\mathrm{JC}} &= \{K(1-3b,b,b,b) \mid b \in [0,1/3]\};\\
\Delta^{\mathrm{JC}}_{\mathrm{dlc}} &= \{K(1-3b,b,b,b) \mid b \in [0,1/4]\};\\
\Delta^{\mathrm{JC}}_{\mathrm{Id}} = \Delta^{\mathrm{JC}}_{\mathrm{emb}} &= \{K(1-3b,b,b,b) \mid b \in [0,1/4)\};\\
\Delta^{\mathrm{JC}}_{\mathrm{dd}} &= \{K(1-3b,b,b,b) \mid b \in [0,1/6]\};
\end{aligned}$$

Using this, it is immediate to check that the space of embeddable Jukes-Cantor matrices has volume (length) 1/4 while the space of all Markov Jukes-Cantor matrices has volume 1/3. Therefore, three out of four Jukes-Cantor matrices are embeddable. Recall that all embeddable JC matrices are also JC-embedable, thus the proportion of embeddable and model-embeddable matrices within JC Markov matrices is the same.

5

EMBEDDABLE MATRICES WHOSE PRINCIPAL LOGARITHM IS NOT A GENERATOR

In this chapter we construct a set with positive measure within the set of 4×4 Markov matrices that contains embeddable matrices whose principal logarithm is *not* a rate matrix. Note that, despite the Markov matrix in Example 4.3.2 is embeddable and its principal logarithm is not a rate matrix, it cannot be perturbed to obtain an open set of matrices satisfying the same. This happens because that matrix has a repeated negative eigenvalue and any open neighbourhood contains Markov matrices with complex non-negative eigenvalues for which the principal logarithm is a rate matrix. Therefore, in order to accomplish the goal of this section it is necessary to look for another class of matrices. In this sense, strand symmetric matrices with a conjugated pair of non-real eigenvalues and positive determinant will work. Recall from Definition 1.4.4 that SS matrices are real and have the following form:

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

In the first section of this chapter we give a necessary condition for the embeddability of (a dense subset of) SS Markov Markov matrices and use the algorithms introduced in Chapter 3 to measure how big the set of embeddable SS matrices is. In the second section we show that there exist *embeddable* SS matrices with different eigenvalues whose *principal logarithm is not a rate matrix*. In the last section, we explain how to deform these examples of SS embedable matrices in order to obtain open subsets in the space of 4×4 Markov matrices formed by embeddable matrices that satisfy the same (see Theorem 5.3.1). Actually, our result proves that for any $k \in \mathbb{Z}$, there is a non-empty open set of embeddable Markov matrices whose unique Markov generator is Log_k (this notation was introduced in (3.1)) .

5.1 THE EMBEDDING PROBLEM FOR SS MARKOV MATRICES

Strand symmetric matrices are not simultaneously diagonalizable and may have non-real eigenvalues. This makes the study of their embeddability is much more complex than for K3P matrices (see Chapter 4). Nevertheless, there is a change of basis that transforms all SS matrices into block-diagonal matrices, which is given by the following transformation matrix

$$S := \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

Lemma 5.1.1 ([CK13, Lemma 6.2] and [JS16])**.** *A matrix $M \in M_4(\mathbb{R})$ is a SS matrix if and only if*

$$S^{-1}MS = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \text{ for some } A, B \in M_2(\mathbb{R}).$$

Proof. This can be proven by direct computation. Indeed,

$$S^{-1}MS = \begin{pmatrix} a+d & b+c & 0 & 0 \\ e+h & f+g & 0 & 0 \\ 0 & 0 & f-g & e-h \\ 0 & 0 & b-c & a-d \end{pmatrix}. \tag{5.1}$$

Furthermore,

$$S \begin{pmatrix} \alpha & \psi & 0 & 0 \\ \kappa & \beta & 0 & 0 \\ 0 & 0 & \delta & \varepsilon \\ 0 & 0 & \phi & \gamma \end{pmatrix} S^{-1} = \frac{1}{2} \begin{pmatrix} \alpha+\gamma & \psi+\phi & \psi-\phi & \alpha-\gamma \\ \kappa+\phi & \delta+\varepsilon & \delta-\varepsilon & \kappa-\phi \\ \kappa-\varepsilon & \beta-\delta & \beta+\delta & \kappa+\varepsilon \\ \alpha-\gamma & \psi-\phi & \psi+\phi & \alpha+\gamma \end{pmatrix}. \qquad \square$$

As in the case of K3P matrices, the structure of SS matrices guarantees that *all* real logarithms of generic SS matrices (that is, with different eigenvalues) are also SS matrices.

Proposition 5.1.2. *Let M be a SS Markov matrix with no repeated eigenvalues. Then, all its real logarithms are SS matrices. In particular, M is embeddable if and only if M is SS-embedable.*

Proof. Since M is a SS matrix with no repeated eigenvalues, it is diagonalizable. By Lemma 5.1.1 we have $M = S\ \mathrm{diag}(A, B)\ S^{-1}$ where A and B are 2×2 diagonalizable real matrices. Take $P_A, P_B \in GL_2(\mathbb{C})$ such that $P_A^{-1} A P_A$ and $P_B^{-1} B P_B$ are diagonal matrices and define the matrix $P = S\mathrm{diag}(P_A, P_B)$. By construction we have that $P^{-1}MP$ is a diagonal matrix. Since M has different eigenvalues, any real matrix Q satisfying $\exp(Q) = M$ can be diagonalized by P (see Remark 1.1.26). Therefore, we have that $S^{-1}QS$ is a block-diagonal matrix and hence Q is a SS matrix by Lemma 5.1.1. □

Remark 5.1.3. This proof is also valid if the eigenvalues of M are 1, 1, μ, $\overline{\mu}$. In this case, M and all its logarithms with rows summing to zero are simultaneously diagonalizable for any $P \in GL_n(\mathbb{C})$ such that $P^{-1}MP$ is a diagonal matrix (see Proposition 3.1.3). In particular, all the real logarithms of M with row sum equal to 0 can be diagonalized by $P = S\mathrm{diag}(P_A, P_B)$. Therefore, all the real logarithms of SS matrices with non-real eigenvalues are also SS matrices.

Next, we focus on the embeddability of SS matrices with non-real eigenvalues. Recall that in Chapter 3, we saw that any Markov generator of such a matrix M is necessarily of the form $\mathrm{Log}_k(M)$ introduced in Section 3.1.2. Moreover, according to Proposition 5.1.2 and Remark 5.1.3 these generators are SS matrices. Below we give an alternative expression for $\mathrm{Log}_k(M)$ that clearly shows its SS structure. To this end, given $v = (v_1, \dots, v_6) \in \mathbb{R}^6$ and $\theta \in \mathbb{R}$ we introduce the matrix $Q(\theta, v)$ defined as follows:

$$\frac{1}{2}\begin{pmatrix} -v_1 - v_3 + \theta v_5 & v_1 - \theta v_4 & v_1 + \theta v_4 & -v_1 + v_3 - \theta v_5 \\ v_2 + \theta v_6 & -v_2 - v_3 - \theta v_5 & -v_2 + v_3 + \theta v_5 & v_2 - \theta v_6 \\ v_2 - \theta v_6 & -v_2 + v_3 + \theta v_5 & -v_2 - v_3 - \theta v_5 & v_2 + \theta v_6 \\ -v_1 + v_3 - \theta v_5 & v_1 + \theta v_4 & v_1 - \theta v_4 & -v_1 - v_3 + \theta v_5 \end{pmatrix}. \quad (5.2)$$

Note that these matrices are SS matrices whose rows sum to zero. Actually, the following lemma shows that any SS matrix with row sums equal to zero is one of these matrices.

Lemma 5.1.4. *Let Q be a SS matrix whose rows sum to 0. Then, for any $\theta \in \mathbb{R}$, $\theta \neq 0$, there exists a unique $v \in \mathbb{R}^6$ such that $Q = Q(\theta, v)$. More precisely,*

$$\begin{aligned} v_1 &= 2(q_{1,2} + q_{1,3}), & v_2 &= 2(q_{2,1} + q_{2,4}), \\ v_3 &= -(q_{2,2} - q_{2,3}) - (q_{1,1} - q_{1,4}), & v_4 &= -\tfrac{2(q_{1,2} - q_{1,3})}{\theta}, \\ v_5 &= \tfrac{-(q_{1,1} - q_{1,4}) - (q_{2,2} - q_{2,3})}{\theta}, & v_6 &= \tfrac{2(q_{2,1} - q_{2,4})}{\theta}. \end{aligned} \tag{5.3}$$

Proof. Using that the rows of $Q = (q_{i,j})$ sum to zero, (5.1) yields

$$Q = S \begin{pmatrix} -q_{1,2} - q_{1,3} & q_{1,2} + q_{1,3} & 0 & 0 \\ q_{2,1} + q_{2,4} & -q_{2,1} + q_{2,4} & 0 & 0 \\ 0 & 0 & q_{2,2} - q_{2,3} & q_{2,1} - q_{2,4} \\ 0 & 0 & q_{1,2} - q_{1,3} & q_{1,1} - q_{1,4} \end{pmatrix} S^{-1}.$$

Analogously, for $Q(\theta, v)$ we have

$$Q(\theta, v) = S \begin{pmatrix} \frac{-v_1}{2} & \frac{v_1}{2} & 0 & 0 \\ \frac{v_2}{2} & \frac{-v_2}{2} & 0 & 0 \\ 0 & 0 & \frac{-v_3 - \theta v_5}{2} & \frac{\theta v_6}{2} \\ 0 & 0 & \frac{-\theta v_4}{2} & \frac{-v_3 + \theta v_5}{2} \end{pmatrix} S^{-1}. \tag{5.4}$$

We obtain (5.3) by imposing $Q = Q(\theta, v)$. □

Note that one can easily compute the eigenvalues of $Q(\theta, v)$ from (5.4). Indeed, we have:

$$\sigma(Q(\theta, v)) = \left\{0, -v_1 - v_2, -v_3 \pm \theta\sqrt{v_5^2 - v_4 v_6}\right\} \tag{5.5}$$

Hence, if $Q(\theta, v)$ has a conjugated-pair of non-real eigenvalue then $v_5^2 - v_4 v_6 < 0$. In this case, the imaginary part of these eigenvalues is equal to $\pm\theta$ provided that v lies in the algebraic variety

$$\mathcal{W} = \{(v_1, \ldots, v_6) \in \mathbb{R}^6 \mid v_4 v_6 - v_5^2 = 1\}.$$

Remark 5.1.5. $\mathcal{W} = \mathbb{R}^3 \times \mathcal{V}$, where $\mathcal{V}$ is the variety defined in (3.4).

Theorem 5.1.6. *Given $\theta \in (-\pi, \pi)$ and $v \in \mathcal{W}$, define $M = \exp(Q(\theta, v))$. Then:*

i) The matrix M is a SS matrix with rows summing to 1.

ii) $\exp(Q(\theta + 2\pi k, v)) = M$ for all $k \in \mathbb{Z}$.

iii) If $\theta \neq 0$, then M has two non-real conjugated pair of eigenvalues $\mu, \overline{\mu}$ whose principal argument is equal to $\pm\theta$. In this case, we have $\mathrm{Log}_k(M) = Q(\theta + 2\pi k, v)$.

Proof.

i) Since $Q(\theta, v)$ is a SS matrix whose rows sum to zero, then $\mathbf{1} = (1,1,1,1)^t$ is an eigenvector of $Q(\theta, v)$ with eigenvalue 0 . From Lemma 1.1.12 we get that $\mathbf{1}$ is also an eigenvector with eigenvalue $e^0 = 1$ of M and hence the rows of M sum to 1. To conclude this part of the proof, note that Lemma 5.1.1 yields that $S^{-1}Q(\theta, v)S$ is a block-diagonal matrix, thus Remark 1.1.8 implies that $\exp(S^{-1}Q(\theta, v)S) = S^{-1}\exp(Q(\theta, v))S$ is also a block-diagonal matrix. Hence, we get that $\exp(Q(\theta, v))$ is a SS matrix by Lemma 5.1.1.

ii) Given $v = (v_1, v_2, v_3, v_4, v_5, v_6) \in \mathcal{W}$, write $w = (0, 0, 0, v_4, v_5, v_6)$. Note that as v lies in $\mathcal{W}$ so does w, thus the eigenvalues of $Q(2\pi k, w)$ are $0, 0, 2\pi k i, -2\pi k i$ (see (5.5)). Hence, Lemma 1.1.12 implies that $\exp(Q(2\pi k, w)) = Id$. Now, $Q(\theta + 2\pi k, v) = Q(\theta, v) + Q(2\pi k, w)$ and it is immediate to check that $Q(\theta, v)$ and $Q(2\pi k, w)$ commute. Indeed, a straightforward computation shows that $Q(\alpha, v)Q(\beta, w) = Q(\beta, w)Q(\alpha, v)$ for any $\alpha, \beta \in \mathbb{C}$. Therefore, Proposition 1.1.14 yields $\exp(Q(\theta + 2\pi k, v)) = \exp(Q(\theta, v))\ \exp(Q(2\pi k, w)) = \exp(Q(\theta, v))$.

iii) According to (5.5), $Q(\theta, v)$ has a conjugated pair of eigenvalues $\mu, \overline{\mu}$ with imaginary part equal to $\pm\theta$. Hence, Lemma 1.1.12 yields that M has a conjugated pair of eigenvalues with principal argument $\pm\theta$. Note that μ and $\overline{\mu}$ are not real because $|\theta| < \pi$ and $\theta \neq 0$. By statement ii) we have that $Q(\theta + 2\pi k, v)$ is a logarithm of M. Actually, (3.1) and (5.5) imply that $Q(\theta + 2\pi k, v) = \mathrm{Log}_k(M)$. □

As a byproduct of the previous results, we can use the same vector $v \in \mathcal{W}$ to express all the Markov generators of any embedabble SS matrix with a given non-real eigenvalue μ with $\mathrm{Im}(\mu) > 0$ as $Q(\mathrm{Arg}(\mu) + 2\pi k, v)$.

Corollary 5.1.7. *Let M be a SS Markov matrix with non-real eigenvalues $1, \lambda, \mu, \overline{\mu}$ with $\lambda \in (0, 1]$, $\mu \in \mathbb{C} \setminus \mathbb{R}$, $\mathrm{Im}(\mu) > 0$. Then, there exists $v \in \mathbb{R}^6$ such that $\mathrm{Log}_k(M) = Q(\mathrm{Arg}(\mu) + 2\pi k, v)$ for all $k \in \mathbb{Z}$. Moreover, v is unique and it lies in $\mathcal{W}$.*

Proof. Proposion 2.3.2 claims that all real logarithms with rows summing to zero of M are of the form $\mathrm{Log}_k(M)$ for some $k \in \mathbb{Z}$. Moreover, all these logarithms are SS matrices by Proposition 5.1.2. Hence, according to Lemma 5.1.4 there is a unique $v \in \mathbb{R}^6$ such that $\mathrm{Log}_0(M) = Q(\mathrm{Arg}(\mu), v)$. Now, recall that $\mathrm{Log}_0(M)$ is the principal logatrithm of M (see Definition 2.3.1), so its eigenvalues are necessarily 0, $\log(\lambda)$, $\log(\mu) + Arg(\mu)i$ and $\log(\mu) - Arg(\mu)i$. The particular form of the eigenvalues of $Q(\mathrm{Arg}(\mu), v)$ in terms of the components v_i (see (5.5)) implies that v lies in $\mathcal{W}$ and from Theorem 5.1.6 ii) we obtain that $Q(\mathrm{Arg}(\mu) + 2\pi k, v) = \mathrm{Log}_k(M)$. □

Next we give a necessary condition for a SS Markov matrix with non-real eigenvalues to be embeddable in terms of its principal logarithm:

Theorem 5.1.8. *Let $M = P\ \mathrm{diag}(1, \lambda, \mu, \overline{\mu})\ P^{-1}$ be a SS Markov matrix with $\lambda \in (0, 1]$, $\mu \in \mathbb{C} \setminus \mathbb{R}$, $\mathrm{Im}(\mu) > 0$, and $P \in GL_4(\mathbb{C})$. If M is embeddable then one of the following does necessarily hold:*

i) $\mathrm{Log}(M)$ *is a rate matrix.*

ii) $\mathrm{Log}(M)$ *has no null entries and exactly two negative off-diagonal entries, which lie in its anti-diagonal.*

Proof. If M is embeddable then there exists a rate matrix $Q = (q_{ij})$ such that $\exp(Q) = M$. By Proposion 2.3.2, there is $k \in \mathbb{Z}$, $k \neq 0$ such that $Q = \mathrm{Log}_k(M)$. Moreover, by Corollary 5.1.7 there is $v \in \mathcal{W}$ such that $Q = Q(\mathrm{Arg}(\mu) + 2\pi k, v)$ is a rate matrix. For such v we have $\mathrm{Log}(M) = Q(\mathrm{Arg}(\mu), v)$ (see Theorem 5.1.6). In particular, $\mathrm{Log}(M)$ is a SS matrix whose rows sum to zero. If $Q = \mathrm{Log}(M)$ then $k = 0$ and i) does hold.

Now, assume that $\operatorname{Log}(M) = (l_{i,j})$ is not a rate matrix. According to (5.2), we have that $q_{1,2} + q_{1,3} = v_1$. Therefore, $v_1 \geq 0$ because the off-diagonal entries of q are non-negative. Since $\operatorname{Arg}(\mu) \in (0, \pi)$ we have that $|\operatorname{Arg}(\mu)| < |\operatorname{Arg}(\mu) + 2\pi k|$ for all $k \neq 0$. Moreover, $v_4, v_6 \neq 0$ because $v \in \mathcal{W}$. Hence, we have that $v_1 \pm (\operatorname{Arg}(\mu) + 2\pi k)v_4 \geq 0$ implies $v_1 \pm \operatorname{Arg}(\mu)v_4 > 0$. Therefore, $q_{1,2}, q_{1,3} \geq 0$ imply that $l_{1,2}, l_{1,3} > 0$. Analogously, from $q_{2,1} + q_{2,4} = v_2$ we deduce that $v_2 \geq 0$ and $l_{2,1}, l_{2,4} > 0$. Moreover, we also have $l_{3,1}, l_{3,4}, l_{4,2}, l_{4,3} > 0$ due to the symmetries of SS matrices. Finally, note that $l_{1,4} + l_{2,3} = q_{1,4} + q_{2,3} \geq 0$. Since L is not a rate matrix this implies that that either $l_{1,4} > 0, l_{2,3} < 0$ or $l_{1,4} < 0, l_{2,3} > 0$. In order to conclude the proof it is enough to note that $l_{1,4} = l_{4,1}$ and $l_{2,3} = l_{3,2}$. Since all off-diagonal entries of Q are different than zero and all its rows sum to zero, we deduce that Q has no null entries. □

Since the space of SS Markov matrices has dimension six, it is not possible to obtain a characterization for the embeddability of SS Markov matrices just in terms of their eigenvalues as we did for K3P matrices (see Section 4.2). Nevertheless, the embeddability of SS Markov matrices can be easily decided by using the algorithms introduced in Section 3.2. Table 5.1 shows the proportion of embeddable SS matrices within the set of all SS Markov matrices Δ and within the relevant subsets introduced in Definition 1.4.11.

	Samples	Embeddable samples	Proportion of embeddable
Δ^{SS}	10^8	174520	0.017452
$\Delta^{\mathrm{SS}}_{\mathrm{Id}}$	4998715	174520	0.034913
$\Delta^{\mathrm{SS}}_{\mathrm{dlc}}$	1021064	173425	0.1698473
$\Delta^{\mathrm{SS}}_{\mathrm{dd}}$	156137	49732	0.3185151

Table 5.1: We sampled 10^8 Markov matrices uniformly and independently from the space of SS Markov matrices. For each of these sets introduced in Definition 1.4.11(Δ^{SS}, $\Delta^{\mathrm{SS}}_{\mathrm{Id}}$, $\Delta^{\mathrm{SS}}_{\mathrm{dlc}}$, $\Delta^{\mathrm{SS}}_{\mathrm{dd}}$), the first column shows how many sample points lie in the set, the second column shows how many of them are embeddable and the third column displays the corresponding proportion. Embeddability was checked with Algorithm 3.2.2.

5.2 STRAND SYMMETRIC MATRICES WHOSE PRINCIPAL LOGARITHM IS NOT A RATE MATRIX

In this section we construct a family of *embeddable* SS matrices with no repeated eigenvalues *whose principal logarithm is not a rate matrix.* In particular, we give a negative answer to Question 3 in the introduction with respect to whether the embeddability of a generic Markov matrix can be decided from its principal logarithm. To this end, we shall use a SS 4×4 matrix M with non-real eigenvalues, so that it has other real logarithms in addition to its principal logarithm (see Proposition 1.3.6). As explained in the previous section, all the real logarithms of M with rows summing to 0 can be written as $\mathrm{Log}_k(M) = Q(\theta_k, v)$ for some $k \in \mathbb{Z}$, $v \in \mathcal{W}$ and $\theta_k \in \mathbb{R}$ (see Corollary 5.1.7). Note that by fixing θ, one can characterize when $Q(\theta, v)$ is a rate matrix in terms of $v \in \mathbb{R}^6$ by solving a system of linear inequalities.

Definition 5.2.1. Given $\theta \in (-\pi, \pi)$, we denote by $\mathcal{R}(\theta)$ the set of those $v \in \mathbb{R}^6$ such that $Q(\theta, v)$ is a rate matrix and by $\mathcal{R}(\theta)^c$ its complementary.

Remark 5.2.2. Since the rows of $Q(\theta, v)$ sum to zero, $\mathcal{R}(\theta)$ is the solution of the inequation system $Q(\theta, v)_{i,j} \geq 0$ for all pairs (i, j) with $i \neq j$. Therefore, $\mathcal{R}(\theta)$ is an unbounded convex polyhedral cone because these inequalites are linear with respect to θ (see (5.2)). In particular, if $Q(\theta, v)$ is a rate matrix so is $Q(\theta, \lambda v)$ for any $\lambda \geq 0$ (see Remark 1.2.13).

Lemma 5.2.3. *For any $\theta \in (-\pi, \pi)$ and any $k \in \mathbb{Z}$, $k \neq 0$, we have that $\mathcal{R}(\theta)^c \cap \mathcal{R}(\theta + 2\pi k)$ has two connected components $\mathcal{C}_1^{(k)}$ and $\mathcal{C}_2^{(k)}$, where $\mathcal{C}_1^{(k)}$ is the set of solutions to the following inequalities:*

$$\begin{aligned} -v_1 + v_3 - \theta v_5 &< 0, \\ -v_1 + v_3 - (\theta + 2\pi k)v_5 &\geq 0, \\ -v_2 + v_3 + (\theta + 2\pi k)v_5 &\geq 0, \end{aligned} \qquad \begin{aligned} v_1 + (\theta + 2\pi k)v_4 &\geq 0, \\ v_1 - (\theta + 2\pi k)v_4 &\geq 0, \\ v_2 + (\theta + 2\pi k)v_6 &\geq 0, \\ v_2 - (\theta + 2\pi k)v_6 &\geq 0. \end{aligned} \tag{5.6}$$

Moreover, $(v_1, v_2, v_3, v_4, v_5, v_6) \in \mathcal{C}_1^{(k)}$ if and only if $(v_2, v_1, v_3, v_6, -v_5, v_4) \in \mathcal{C}_2^{(k)}$.

Proof. Recall that $Q(\theta, v)$ is a SS matrix and hence it is enough to look at its first two rows to decide if it is a rate matrix or not. Let us take $v \in \mathcal{R}(\theta)^c \cap \mathcal{R}(\theta + 2\pi k)$, so that $R := Q(\theta + 2\pi k, v)$ is a rate matrix while $L := Q(\theta, v)$ is not. By Theorem 5.1.6 we have $\exp(R) = \exp(L)$. Moreover, $\exp(R)$ is an embeddable matrix (because R is a rate matrix) and $L = (l_{ij})$ is its principal logarithm. By construction L is not a rate matrix, thus Theorem 5.1.8 implies that either $l_{1,4} \geq 0,\ l_{2,3} < 0$ or $l_{2,3} \geq 0,\ l_{1,4} < 0$. This proves that $\mathcal{R}(\theta)^c \cap \mathcal{R}(\theta + 2\pi k)$ has two connected components. The system of linear inequalities in (5.6) is the reduced system arising from the assumption that the only negative off-diagonal entry of R and L is $l_{1,4}$. We denote this component by $\mathcal{C}_1^{(k)}$. In order to conclude the proof, consider the vectors $v = (v_1, v_2, v_3, v_4, v_5, v_6)$ and $\widetilde{v} = (v_2, v_1, v_3, v_6, -v_5, v_4)$. From the definition of $Q(\theta, v)$ in (5.2) one can immediately check that $Q(\theta, v)$ and $Q(\theta, \widetilde{v})$ have the same off-diagonal entries (in different order). Moreover, $Q(\theta, v)_{1,4} = Q(\theta, \widetilde{v})_{2,3}$ and $Q(\theta, v)_{2,3} = Q(\theta, \widetilde{v})_{1,4}$ so that $v \in \mathcal{C}_1^{(k)}$ if and only if $\widetilde{v} \in \mathcal{C}_2^{(k)}$. □

Note that given $v \in \mathcal{C}_1^{(k)} \cap \mathcal{W}$, Theorem 5.1.6 gives that

$$M = \exp(Q(\theta, v)) = \exp(Q(\theta + 2\pi k, v))$$

is a SS matrix. Moreover, by construction we have that $Q(\theta + 2\pi k, v)$ is a rate matrix and hence M is an embeddable SS matrix (see Theorem 1.2.12). However, $\mathrm{Log}(M) = Q(\theta, v)$ is not a rate matrix because $v \in \mathcal{R}^c(\theta)$. Therefore, we have a constructive method to obtain embeddable SS matrices whose principal logarithm is not a rate matrix.

Example 5.2.4. For each $k \neq 0$ we construct an example of an embeddable SS matrix whose unique Markov generator is Log_k. This family of examples is obtained by taking $M = \exp(Q(\theta, v))$ with $\theta = \pi/2$ and

$$v = \left(3|\theta + 2\pi k| + \frac{\pi}{2}, |\theta + 2\pi k| + \frac{\pi}{2}, 2|\theta + 2\pi k| + \pi, -2, -sign(k), -1\right).$$

This vector lies in the interior of $\mathcal{C}_1^{(k)} \cap \mathcal{W}$ and has been obtained using the mathematical software Maple [Map09].

- For $k \in \mathbb{Z}_{\geq 0}$, consider the Markov matrix given by $M = P_+ \, D_+ \, P_+^{-1}$ where $D_+ := \text{diag}(1, e^{(1-8k)\pi}, e^{-2\pi(1+2k)}i, -e^{-2\pi(1+2k)}i)$ and

$$P_+ := \begin{pmatrix} 1 & 6k+2 & 1-i & 1+i \\ 1 & -2k-1 & -i & +i \\ 1 & -2k-1 & i & +i \\ 1 & 6k+2 & -1+i & -1-i \end{pmatrix}.$$

A straightforward computation shows that M is a Markov matrix. Further computations show that, for any $l \in \mathbb{Z}$, the matrix $\text{Log}_l(M)$ is equal to

$$\frac{\pi}{4}\begin{pmatrix} -9-20k-4l & 6+12k+8l & 2+12k-8l & 1-4k+4l \\ 1+4k-4l & -5-12k+4l & 1+4k-4l & 3+4k+4l \\ 3+4k+4l & 1+4k-4l & -5-12k+4l & 1+4k-4l \\ 1-4k+4l & 2+12k-8l & 6+12k+8l & -9-20k-4l \end{pmatrix}.$$

Since $l, k \in \mathbb{Z}$ and $k \geq 0$, the only possible choice for l so that all off-diagonal entries are non-negative is $l = k$ (this can be easily seen by looking at the entries $(2,1)$ and $(4,1)$ for instance). In this case we have:

$$\text{Log}_k(M) = \frac{\pi}{4}\begin{pmatrix} -9-24k & 6+20k & 2+4k & 1 \\ 1 & -5-8k & 1 & 3+8k \\ 3+8k & 1 & -5-8k & 1 \\ 1 & 2+4k & 6+20k & -9-24k \end{pmatrix}.$$

- For $k \in \mathbb{Z}_{<0}$, consider the Markov matrix given by $M = P_- \, D_- \, P_-^{-1}$ where $D_- := \text{diag}(1, e^{(1+8k)\pi}, e^{4k\pi}i, -e^{4k\pi}i)$ and

$$P_- := \begin{pmatrix} 1 & 6k+1 & 1-i & 1+i \\ 1 & -2k & -i & i \\ 1 & -2k & i & -i \\ 1 & 6k+1 & -1+i & -1-i \end{pmatrix}.$$

In this case, given $l \in \mathbb{Z}$ we have that the matrix $\text{Log}_l(M)$ is equal to

$$\frac{\pi}{4}\begin{pmatrix} 3+20k+4l & -12k+8l & -4-12k-8l & 1+4k-4l \\ -1-4k-4l & -1+12k-4l & 1-4k+4l & 1-4k+4l \\ 1-4k+4l & 1-4k+4l & -1+12k-4l & -1-4k-4l \\ 1+4k-4l & -4-12k-8l & -12k+8l & 3+20k+4l \end{pmatrix}.$$

Since $l, k \in \mathbb{Z}$ and $k < 0$, the only possible choice for l that produces only non-negative off-diagonal entries is $l = k$. Indeed,

$$\mathrm{Log}_k(M) = \frac{\pi}{4}\begin{pmatrix} 3+24k & -4k & -4-20k & 1 \\ -1-8k & -1+8k & 1 & 1 \\ 1 & 1 & -1+8k & -1-8k \\ 1 & -4-20k & -4k & 3+24k \end{pmatrix}.$$

In both cases, the given Markov matrix M is *embeddable* and $\mathrm{Log}_k(M)$ is its *unique* Markov generator.

For $k \neq 0$, the matrices described in the previous example are embeddable matrices whose principal logarithm is not a rate matrix. Up to our knowledge, these are the first known examples of embeddable matrices with different eigenvalues satisfying this property (cf. Example 4.3.2). According to Theorem 1.3.14, if $k \neq 0$ and $k \neq -1$, there is no analogous construction for 3×3 Markov matrices.We conclude this section by giving explicitly the matrix M for $k = 1$.

Example 5.2.5. Rounding to the 10-th decimal and taking $k = 1$ the matrix M in the previous example is:

$$M = \begin{pmatrix} 0.1363636331 & 0.3636363701 & 0.3636363571 & 0.1363636397 \\ 0.1363636331 & 0.3636363669 & 0.3636363603 & 0.1363636397 \\ 0.1363636397 & 0.3636363603 & 0.3636363669 & 0.1363636331 \\ 0.1363636397 & 0.3636363571 & 0.3636363701 & 0.1363636331 \end{pmatrix}.$$

In this case, M is an embeddable SS matrix whose principal logarithm is not a rate matrix and whose only generator is $\mathrm{Log}_1(M)$.

$$\mathrm{Log}(M) = \frac{\pi}{4}\begin{pmatrix} -29 & 18 & 14 & -3 \\ 5 & -17 & 5 & 7 \\ 7 & 5 & -17 & 5 \\ -3 & 14 & 18 & -29 \end{pmatrix}$$

and

$$\mathrm{Log}_1(M) = \frac{\pi}{4}\begin{pmatrix} -33 & 26 & 6 & 1 \\ 1 & -13 & 1 & 11 \\ 11 & 1 & -13 & 1 \\ 1 & 6 & 26 & -33 \end{pmatrix}.$$

5.3 AN OPEN SET OF EMBEDDABLE MATRICES WHOSE UNIQUE LOGARITHM IS Log_k

In this section we perturb the entries of the matrices obtained in Example 5.2.4 in order to obtain embeddable matrices (with no symmetry constraints) whose unique Markov generator is still the logarithm Log_k defined in (3.1).

Theorem 5.3.1. *For any $k \in \mathbb{Z}$, there is a non-empty Euclidean open set of embeddable Markov matrices whose unique Markov generator is given by Log_k. In particular, there is a non-empty Euclidean open set of 4×4 Markov matrices that are embeddable and whose principal logarithm is not a rate matrix.*

Proof. Let us define the matrix

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & i & -i \end{pmatrix}.$$

Given $\varepsilon = (\varepsilon_1, \dots, \varepsilon_{12}) \in \mathbb{R}^{12}$ consider the matrix

$$A_\varepsilon = \begin{pmatrix} 1 & \varepsilon_1 & \varepsilon_4 & \varepsilon_7 \\ 0 & 1 & \varepsilon_5 & \varepsilon_8 \\ 0 & \varepsilon_2 & 1 & \varepsilon_9 \\ 0 & \varepsilon_3 & \varepsilon_6 & 1 \end{pmatrix}.$$

Now, taking P_+ and P_- as in Example 5.2.4 we define the matrices H and D_ε depending on the sign of k as follows:

- If $k \in \mathbb{Z}_{\geq 0}$, take $H = P_+ \, R^{-1} = \begin{pmatrix} 1 & 6k+2 & 1 & -1 \\ 1 & -2k-1 & 0 & -1 \\ 1 & -2k-1 & 0 & 1 \\ 1 & 6k+2 & -1 & 1 \end{pmatrix}$,

  $D_\varepsilon = \mathrm{diag}\big(\ 1\ ,\ (1+\varepsilon_{10})e^{(1-8k)\pi}\ ,\ \varepsilon_{11} + i(1+\varepsilon_{12})e^{-2\pi(1+2k)}\ ,\ \varepsilon_{11} - i(1+\varepsilon_{12})e^{-2\pi(1+2k)}\ \big)$.

  Note that $\det(H) = 32k - 12 \neq 0$, so H is invertible.

- If $k \in \mathbb{Z}_{<0}$, take $H = P_-\ R^{-1} = \begin{pmatrix} 1 & 6k+1 & 1 & -1 \\ 1 & -2k & 0 & -1 \\ 1 & -2k & 0 & 1 \\ 1 & 6k+1 & -1 & 1 \end{pmatrix}$,

  $D_\varepsilon = \mathrm{diag}\big(\ 1\ ,\ (1+\varepsilon_{10})e^{(1+8k)\pi}\ ,\ \varepsilon_{11} + i(1+\varepsilon_{12})e^{-4k\pi}\ ,\ \varepsilon_{11} - i(1+\varepsilon_{12})e^{-4k\pi}\ \big)$.

  Analogously to the previous case, $\det(H) = 32k - 4 \neq 0$ and H is invertible.

Next, we need to introduce some notation. We write $U \subset M_4(\mathbb{R})$ for the open set of matrices with non-zero entries and at least one negative entry outside the diagonal, and we write $V \subset M_4(\mathbb{R})$ for the open set of matrices with non-zero entries and positive off-diagonal entries. Given $\kappa > 0$, we write

$$X = \big\{\varepsilon = (\varepsilon_1, \ldots, \varepsilon_{12}) : |\varepsilon_i| < \kappa \text{ for } i = 1, \ldots, 12\big\} \subseteq \mathbb{R}^{12}.$$

Claim 1. *There is $\kappa \in (0,1)$ such that $M_\varepsilon := (HA_\varepsilon R)\ D_\varepsilon\ (HA_\varepsilon R)^{-1}$ is a Markov matrix with positive determinant for all $\varepsilon \in \mathbb{R}^{12}$ satisfying $\varepsilon_i < \kappa$, $i = 1, \ldots, 12$. In this case, M_ε has pairwise different eigenvalues and two of them are non-real.*

For ease of reading we shall prove this claim after finishing the current proof. Take $\kappa \in (0,1)$ as in Claim 1. Note that, if $\varepsilon \in X$, then any real logarithm of M_ε with rows summing to zero is of the form $\mathrm{Log}_l(M_\varepsilon)$ for some $l \in \mathbb{Z}$ (see Section 3.1.2). Now, let $\mathcal{M}_\mathbf{1}$ be the set of 4×4 real matrices with rows summing to one and consider the map $f : X \to \mathcal{M}_\mathbf{1}$ defined by $f(\varepsilon) = M_\varepsilon$. Then, for $m = k-1, k, k+1$ we define the maps $g_m : f(X) \longrightarrow M_4(\mathbb{R})$ by $g_m(M) := \mathrm{Log}_m(M)$. Note that $f(0)$ is the matrix M in Example 5.2.4 and hence $g_{k-1}(f(0)), g_{k+1}(f(0)) \in U$ and $g_k(f(0)) \in V$. Moreover, since f, g_{k-1}, g_k and g_{k+1} are continuous on their respective domains, we have that $g_{k-1}^{-1}(U)$, $g_k^{-1}(V)$ and $g_{k+1}^{-1}(U)$ are open sets in $f(X)$ containing $f(0)$. Therefore,

$$W := g_{k-1}^{-1}(U) \cap g_k^{-1}(V) \cap g_{k+1}^{-1}(U) \subseteq f(X) \tag{5.7}$$

is a non-empty open set in $f(X)$ (it contains $f(0)$). Note that any $M \in W$ is a Markov matrix by Claim 1. Furthermore, according to (5.7) we have that $\mathrm{Log}_k(M)$ is a rate matrix while $\mathrm{Log}_{k-1}(M)$ and $\mathrm{Log}_{k+1}(M)$ are not. Therefore, Lemma 3.1.5 yields that any matrix in W is an embeddable Markov matrix whose only Markov generator is $\mathrm{Log}_k(M)$.

Figure 5.1 illustrates the remaining part of this proof. We shall use the claim below in order to check that W contains a non-empty *open* subset of $\mathcal{M}_{\mathbf{1}}$ and conclude the proof. The proof of this claim can be found after this proof.

Claim 2. *Consider the set $Y = \{\varepsilon \in X \mid \varepsilon_6 + \varepsilon_9 = 0\}$. Then, f is injective in $X \setminus Y$.*

From the claim and the fact that f is continuous on its whole domain we have that $f|_{X\setminus Y} : X \setminus Y \to \mathcal{M}_{\mathbf{1}}$ is a continuous *injective* map. Moreover, since $X \setminus Y$ is open in $\mathbb{R}^{12} \simeq \mathcal{M}_{\mathbf{1}}$ we can apply the invariance of domain theorem to infer that $f|_{X\setminus Y}$ is a homeomorphism from $X \setminus Y$ into its image. Therefore, $f(X \setminus Y)$ is an open set of $\mathcal{M}_{\mathbf{1}}$ and hence so is $f(X \setminus Y) \cap W$. We conclude the proof by showing that $f(X \setminus Y) \cap W \neq \emptyset$. We have that the complementary set of $f(Y)$ is dense in $f(X)$ because $f(Y)$ is an open set of an affine algebraic variety of dimension ≤ 11. This implies that $f(0)$ is adherent to $f(X) \setminus f(Y) \subseteq f(X \setminus Y)$. Therefore, $f(X \setminus Y)$ cuts the neighbourhood W of $f(0)$. □

Proof of Claim 1. By construction, the eigenvalues of M_ε are the diagonal entries in D_ε and the corresponding eigenvectors are the columns of $P_\varepsilon := H\ A_\varepsilon\ R$. Since $\varepsilon \in X$, we have that M_ε is non-singular. Indeed, the first eigenvalue of M_ε is equal to 1 and the second one $(1+\varepsilon_{10})e^{(1-8|k|)\pi}$ is positive. Similarly, the third and fourth eigenvalues and eigenvectors are a conjugated pair. Since H and A_ε are real matrices and the third and fourth columns of R are a conjugated pair of vectors we deduce that M_ε is a real matrix. Moreover, it is immediate to check that the first column of P_ε is the vector $\mathbf{1}$ and hence the rows of M_ε sum to one. Now, note that M_0 is the Markov matrix M in Example 5.2.4, thus M_0 is positive. Therefore, for κ small enough we have that M_ε is a non-negative real matrix with rows summing to one. $\varepsilon \in X$ □

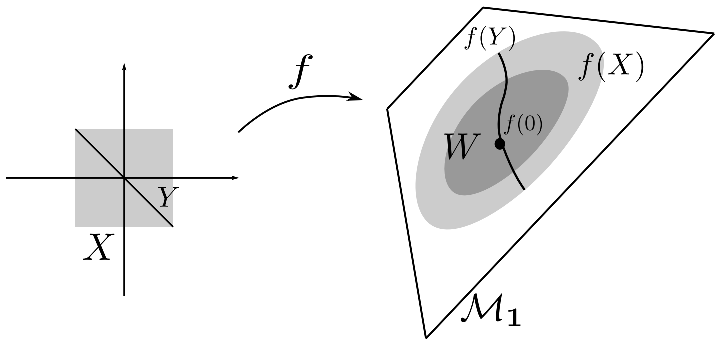

Figure 5.1: This figure illustrates the proof of Theorem 5.3.1. The map $f(\varepsilon) = M_\varepsilon$ is injective in $X \setminus Y$ and $f(0)$ is the matrix M in Example 5.2.4. W is an open set of embeddable $n \times n$ matrices whose principal logarithm is not a rate matrix.

Proof of Claim 2. Since the eigenvalues of any M_ε are all simple, the values of $\varepsilon_{10}, \varepsilon_{11}, \varepsilon_{12}$ are completely determined by M_ε. It remains to see that M_ε also determines the other values of ε_i, $i = 1, \dots, 9$ as long as $\varepsilon \in X \setminus Y$. Let c_i denote the i-th column of A_ε. By construction, the columns of $P_\varepsilon = H\ A_\varepsilon\ R$ are eigenvectors of M_ε, which we proceed to describe now:

- $v_1 = (1, 1, 1, 1)^t$, with eigenvalue $\lambda_1 = 1$.
- $v_2 = Hc_2$, with positive eigenvalue $\lambda_2 = \begin{cases} (1+\varepsilon_{10})e^{(1-8k)\pi} & \text{if } k \geq 0, \\ (1+\varepsilon_{10})e^{(1+8k)\pi} & \text{if } k < 0. \end{cases}$
- $v_3 = H(c_3 + c_4\ i)$, with complex eigenvalue with positive imaginary part
$$\lambda_3 = \begin{cases} \varepsilon_{11} + i(1+\varepsilon_{12})e^{-2\pi(1+2k)} & \text{if } k \geq 0, \\ \varepsilon_{11} + i(1+\varepsilon_{12})e^{-4k\pi} & \text{if } k < 0. \end{cases}$$
- $v_4 = H(c_3 - c_4\ i)$, with complex eigenvalue with negative imaginary part
$$\lambda_4 = \overline{\lambda_3} = \begin{cases} \varepsilon_{11} - i(1+\varepsilon_{12})e^{-2\pi(1+2k)} & \text{if } k \geq 0, \\ \varepsilon_{11} - i(1+\varepsilon_{12})e^{-4k\pi} & \text{if } k < 0. \end{cases}$$

Assume that there are $\varepsilon, \widetilde{\varepsilon} \in X \backslash Y$ so that $M_\varepsilon = M_{\widetilde{\varepsilon}}$ and write $\widetilde{v_1},\ \widetilde{v_2},\ \widetilde{v_3},\ \widetilde{v_4}$ for the corresponding eigenvectors of $M_{\widetilde{\varepsilon}}$ and $\widetilde{c_i}$ for the i-th column of $A_{\widetilde{\varepsilon}}$. Using again that the eigenvalues are simple, we have that there are $z_2, z_3, z_4 \in \mathbb{C}$ such that $v_i = z_i\, \widetilde{v_i},\ i = 2, 3, 4$.

- From $v_2 = z_2\, \widetilde{v_2}$, we have that $Hc_2 = z_2 H\widetilde{c_2} = H\,(z_2\, \widetilde{c_2})$ and hence we get $c_2 = z_2\, \widetilde{c_2}$. From the second component of c_2 and $\widetilde{c_2}$, we deduce that $z_2 = 1$. Hence, $c_2 = \widetilde{c_2}$ which implies that $\varepsilon_i = \widetilde{\varepsilon_i}$ for $i = 1, 2, 3$.

- From $v_3 = z_3\, \widetilde{v_3}$, we deduce that $H(c_3 + c_4\ i) = z_3 H(\widetilde{c_3} + \widetilde{c_4}\ i) = Hz_3(\widetilde{c_3} + \widetilde{c_4}\ i)$, and hence $c_3 + c_4\ i = z_3\ (\widetilde{c_3} + \widetilde{c_4}\ i)$. Write $z_3 = a + bi$ with $a, b \in \mathbb{R}$. By looking at the real part of the third component we get $1 = a - b\widetilde{\varepsilon_9}$. Similarly, from the imaginary part of the fourth component we have $1 = a + b\widetilde{\varepsilon_6}$. Since, $(\widetilde{\varepsilon_9} + \widetilde{\varepsilon_6}) \neq 0$ this implies that $b = 0$ and $a = 1$, so $z_3 = 1$. We derive that $c_3 = \widetilde{c_3}$ and $c_4 = \widetilde{c_4}$ which implies that $\varepsilon_i = \widetilde{\varepsilon_i}$ for $i = 4, \ldots, 9$.

We conclude that $\varepsilon = \widetilde{\varepsilon}$. □

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A

APPENDIX: PYTHON SCRIPTS

Required packages:

```
import numpy as np
from numpy import linalg as la
from scipy import linalg as si
from sympy import *
import math
import cdd
import random
```

Auxiliar functions

```
def GetRandomRow(fineness):
#Input: number of possible values for each number.
#Output: 4 numbers that sum to 1. Obtained by sampling
   uniformly in a grid on a 3-dimensional probability simplex.
    x,y,z= tuple(sorted(random.sample(list(range(fineness+3)),
     3)))
    a=x/fineness
    b=(y-x-1)/fineness
    c=(z-y-1)/fineness
    d=(fineness+2 -z)/fineness
    return a,b,c,d
```

```
def checkRate(Q):
#Input: A real square matrix.
#Output: True if its a rate matrix, False otherwise.
    for i in range(4):
        for j in range(4):
            if Q[i][j]< 0 and i!=j:
                return False
    return True
```

```
def ComplexEmbeddability(LogM,vaps, P):
#Input: Principal logarithm, eigenvalues and eigenvectors of a
     Markov matrix with a conjugated-pair of non real
    eigenvalues.
#Output: List of Markov generators

    output=[]
    Pinv = la.inv(P)

    #Define V depending on the ordering of the eigenvalues.
    if vaps[3].imag != 0:
        if vaps[2].imag != 0:
            aux = P@ np.diag([0,0,np.pi*2j,-np.pi*2j])@Pinv
        elif vaps[1].imag != 0:
            aux = P@ np.diag([0,np.pi*2j,0,-np.pi*2j])@Pinv
        else:
            aux = P@ np.diag([np.pi*2j,0,0,-np.pi*2j])@Pinv
    elif vaps[2].imag != 0:
        if vaps[1].imag != 0:
            aux = P@ np.diag([0,np.pi*2j,-np.pi*2j,0])@Pinv
        else:
            aux = P@ np.diag([0,np.pi*2j,0,-np.pi*2j,0])@Pinv
    else:
        aux = P@ np.diag([np.pi*2j,-np.pi*2j,0,0])@Pinv

    #If det(M) is close to 0, there might be small errors in P
    . As a consequence, the obtained matrix V could have non-
    real entries with a small (O(10^(-16)) imaginary part.
    V= np.zeros((4,4))
    for i in range(4):
        for j in range(4):
            V[i][j]= aux[i][j].real

    #V has at least a negative off-diagonal entry and a
    positive off-diagonal entry so L and U are bounded.
    U=oo
    L=-oo
    for i in range(4):
        for j in range(4):
            if i!= j:
                if V[i][j]> 0:
                    if (-LogM[i][j]/V[i][j] > L):
```

```
                    L=-LogM[i][j]/V[i][j]
                elif V[i][j]<0:
                    if (-LogM[i][j]/V[i][j] < U):
                        U=-LogM[i][j]/V[i][j]
                elif LogM[i][j] < -epsilon:
                    #In this case M is not embeddable.
                    return output
    L= math.ceil(L)
    U= math.floor(U)

    #List of all generators
    if L <= U:
        while L <= U:
            output.append(LogM+L*V)
            L = L+1
    return output
```

Implementation of Algorithm 3.2.2:

```
def CheckEmbeddability(M):
#Input: A Markov matrix with different eigenvalues.
#Output: Its Markov generators (or an empty list).

    #Compute eigenvalues(vaps) and eigenvectors(matrix P) and
    check whether there is a negative or non-real eigenvalue.
    We also check if M has different eigenvalues.
    vaps, P = la.eig(M)
    complexFlag=False
    for i in range(4):
        if vaps[i].imag != 0:
            complexFlag=True
        elif vaps[i] <= 0:
            print("M has a negative or null eigenvalue.")
            return []
        for j in range(4):
            if i!=j and abs(vaps[i]-vaps[j])==0 and vaps[i
    ]!=1:
                print("M has a repeated eigenvalue (!=1).")
                return []

    #If det(M) is close to 0, the matrix LogM might have non-
    real entries with small imaginary components (O(10^-16)).
    LogM = si.logm(M)
```

```
    for i in range(4):
        for j in range(4):
            if LogM[i][j].imag!=0:
                print("Unable to compute Log(M) correctly.")
                return []

    #Compute Markov generators
    if complexFlag:
        return ComplexEmbeddability(LogM,vaps,P)
    elif checkRate(LogM):
        return [LogM]
```

Script used to obtain Table 3.1:

```
#Counters for different cases
Embed=0
DLC=0
DD=0
Repeated=0
Complex=0
sing=0
DLCE=0
DDE=0
ComplexE=0
errorCount=0
n=0
PosDet=0

prec=10000 #Fineness used in GetRandomRow
size=10000000 #Number of samples
InitialTime=time.time()

while n < size:
    #Increase sample counter and reset flags
    n=n+1
    DLCflag= False
    negFlag=False
    DDflag=False
    complexFlag=False
    repeatedFlag=False
    errorFlag=False

    #Generate random Markov matrix
```

```
M= [[0,0,0,0],[0,0,0,0],[0,0,0,0],[0,0,0,0]]
for j in range(4):
    M[j][0],M[j][1],M[j][2],M[j][3]= GetRandomRow(prec)

#Check if M is diagonally dominant or diagonal largest in
column.
if  M[0][0]>=0.5 and M[1][1]>=0.5 and M[2][2]>=0.5 and M
[3][3]>=0.5:
    DD=DD+1
    DLC=DLC+1
    DDflag = True
    DLCflag = True
elif M[0][0]>=M[1][0] and M[0][0]>=M[2][0] and M[0][0]>=M
[3][0] and M[1][1]>=M[0][1] and M[1][1]>=M[2][1] and M
[1][1]>=M[3][1] and M[2][2]>=M[0][2] and M[2][2]>=M[1][2]
and M[2][2]>=M[3][2] and M[3][3]>=M[0][3] and M[3][3]>=M
[1][3] and M[3][3]>=M[2][3]:
    DLCflag=True
    DLC=DLC+1

#Compute eigenvalues (vaps), a basis of eigenvectors (
matrix P) and determinant (det). We check whether there is
any negative or non-real eigenvalue.
vaps, P = la.eig(M)
det=1
for i in range(4):
    det=det*vaps[i]
    if vaps[i].imag != 0:
        complexFlag=True
    elif vaps[i] < 0:
        negFlag=True
    for j in range(4):
        if i!=j and abs(vaps[i]-vaps[j])==0:
            repeatedFlag=True

#If there is a repeated eigenvalue we are not able to test
 all the Markov generators candidates with this algorithm,
in this case the sample is discarded.
if repeatedFlag:
    n=n-1
    repeated=repeated+1
    if DLCFlag:
```

```
            DLC=DLC-1
        if DDFlag:
            DD=DD-1

    #If there is a non-repeated negative eigenvalue the matrix
     is not embeddable.
    elif negFlag:
        if complexFlag:
            Complex=Complex+1

    #Singular matrices have no logarithm (not embeddable).
    elif det == 0:
        sing=sing+1

    elif det>0:
        PosDet=PosDet+1
        LogM = si.logm(M)

        #If det(M) is close to 0, the matrix LogM might have
    non-real entries with small (O(10^-16)) imaginary
    components. In this case, the sample is discarded.
        for i in range(4):
                for j in range(4):
                    if LogM[i][j].imag!=0:
                        errorFlag = True
        if errorFlag:
            errorCount=errorCount+1
            n=n-1
            if DLCFlag:
                DLC=DLC-1
                if DDFlag:
                DD=DD-1

        #Check embeddability
        elif complexFlag:
            Complex=Complex+1
            generators = ComplexEmbeddability(LogM,vaps,P)
            if generators != []:
                Embed=Embed+1
                if DLCflag:
                    DLCE=DLCE+1
                if DDflag:
```

```
                    DDE=DDE+1
                ComplexE=ComplexE+1
        elif checkRate(LogM):
            Embed=Embed+1
            if DLCflag:
                DLCE=DLCE+1
            if DDflag:
                DDE=DDE+1

#Output.
print("\nNUMBER OF SAMPLES:","\n Total:",size,"\n", "
    Embeddable:",Embed,"\n", "DLC",DLC,"\n", "DD", DD,"\n", "
    Positive Determinant:", PosDet, "\n", "Complex eigenvalues:
    ", Complex)
print("\nNUMBER OF EMBEDDABLE SAMPLES:\n","Total:",Embed, "\n
    DLC", DLCE,"\n DD:",DDE,"\n Complex",ComplexE)
print("\n \nSpecial Cases \nRepeated and Singular:", Repeated
    , sing)
print("Total time:",time.time()-InitialTime)
print("Error", errorCount)
```

Script used to obtain Table 5.1:

```
#Counters for different cases
Embed=0
DLC=0
DD=0
Repeated=0
Complex=0
sing=0
DLCE=0
DDE=0
ComplexE=0
errorCount=0
n=0
PosDet=0

prec=10000000 #Fineness used in GetRandomRow
size=10000000 #Number of samples
InitialTime=time.time()

while n < size:
    #Increase sample counter and reset flags
```

```
    n=n+1
    DLCflag= False
    negFlag=False
    DDflag=False
    complexFlag=False
    repeatedFlag=False
    errorFlag=False

    #Generate random SS matrix
    M= [[0,0,0,0],[0,0,0,0],[0,0,0,0],[0,0,0,0]]
    for i in range(2):
        M[i][0],M[i][1],M[i][2],M[i][3]= GetRandomRow(prec)
    for i in range(2):
        for j in range(4):
                M[3-i][3-j]= M[i][j]

    #Check if M is diagonally dominant or diagonal largest in
   column.
    if  M[0][0]>=0.5 and M[1][1]>=0.5:
        DD=DD+1
        DLC=DLC+1
        DDflag = True
        DLCflag = True
    elif M[0][0]>=M[1][0] and M[0][0]>=M[2][0] and M[0][0]>=M
   [3][0] and M[1][1]>=M[0][1] and M[1][1]>=M[2][1] and M
   [1][1]>=M[3][1]:
        DLCflag=True
        DLC=DLC+1

    #Compute eigenvalues (vaps), a basis of eigenvectors (
   matrix P) and determinant (det). We check whether there is
   any negative or non-real eigenvalue.
    vaps, P = la.eig(M)
    det=1
    for i in range(4):
        det=det*vaps[i]
        if vaps[i].imag != 0:
            complexFlag=True
        elif vaps[i] < 0:
            negFlag=True
        for j in range(4):
            if i!=j and abs(vaps[i]-vaps[j])==0:
```

```
            repeatedFlag=True

        #If there is a repeated eigenvalue we are not able to
test all the Markov generators candidates with this
algorithm, in this case the sample is discarded.
        if repeatedFlag:
        n=n-1
        repeated=repeated+1
        if DLCFlag:
            DLC=DLC-1
        if DDFlag:
            DD=DD-1

    #If there is a non-repeated negative eigenvalue the matrix
     is not embeddable.
    elif negFlag:
        if complexFlag:
            Complex=Complex+1

    #Singular matrices have no logarithm (not embeddable).
    elif det == 0:
        sing=sing+1

    elif det>0:
        PosDet=PosDet+1
        LogM = si.logm(M)

        #If det(M) is close to 0, the matrix LogM might have
non-real entries with small (O(10^-16)) imaginary
components. In this case, the sample is discarded.
        for i in range(4):
                for j in range(4):
                    if LogM[i][j].imag!=0:
                        errorFlag = True
        if errorFlag:
            errorCount=errorCount+1
            n=n-1
            if DLCFlag:
                DLC=DLC-1
                if DDFlag:
                DD=DD-1
```

```
        #Check embeddability
        elif complexFlag:
            Complex=Complex+1
            generators = ComplexEmbeddability(LogM,vaps,P)
            if generators != []:
                Embed=Embed+1
                if DLCflag:
                    DLCE=DLCE+1
                if DDflag:
                    DDE=DDE+1
                ComplexE=ComplexE+1
        elif checkRate(LogM):
            Embed=Embed+1
            if DLCflag:
                DLCE=DLCE+1
            if DDflag:
                DDE=DDE+1


#Output
print("\nNUMBER OF SAMPLES:","\n Total:",size,"\n", "
    Embeddable:",Embed,"\n", "DLC",DLC,"\n", "DD", DD,"\n", "
    Positive Determinant:", PosDet, "\n", "Complex eigenvalues:
    ", Complex)
print("\nNUMBER OF EMBEDDABLE SAMPLES:\n","Total:",Embed, "\n
    DLC", DLCE,"\n DD:",DDE,"\n Complex",ComplexE)
print("\nRELATIVE VOLUME OF EMBEDDABLE\n", "SS", Embed/size, "
    \n DLC", DLCE/DLC,"\n DD:",DDE/DD,"\n Positive Determinant:
    ", Embed/PosDet,"\n Complex",ComplexE/Complex)
print("\n \nSpecial Cases \nRepeated and Singular:", Repeated
    , sing)
print("Total time:",time.time()-InitialTime)
print("Error", errorCount)
```

B

APPENDIX: RESUM EN CATALÀ

B.1 INTRODUCCIÓ

L'objectiu d'aquesta tesi és resoldre el problema d'*embedding* per a matrius de Markov, proposat per Gustav Elfving el 1937 [Elf37]. Una *matriu de Markov* és una matriu quadrada, no negativa i amb files que sumen 1. Diem que una matriu de Markov M és *embeddable* si es pot expressar com l'exponencial d'una *matriu de taxes*, és a dir, si és l'exponencial d'una matriu real, amb files que sumen 0 i amb entrades no negatives fora de la diagonal. En aquest cas, diem que la matriu de taxes és un *generador de Markov* d'M. Tal i com el seu nom indica, el problema d'embedding consisteix a caracteritzar les matrius de Markov que són embeddables.

Objectiu 1 (*Problema d'embedding* [Elf37])**:** Donada M una matriu de Markov, decidir si és embeddable o no.

La motivació del problema ve dels processos de Markov, els quals s'utilitzen per a modelar els canvis d'estat d'una variable aleatòria al llarg del temps sota la hipòtesi que el futur és independent del passat, és a dir, que les probabilitats de substitució entre estats no depenen dels canvis que hagin passat anteriorment. En aquest context, les matrius de Markov també s'anomenen matrius de transició, ja que les seves entrades són les probabilitats de substitució entre estats després d'un període de temps fixat. Quan es considera que aquestes entrades són funcions contínues (i derivables) que depenen del temps, el procés de Markov es pot descriure en termes de les taxes instantànies de substitució entre estats. Per tal de mantenir el processos en temps continu tractables, sovint es considera que les taxes de substitució instantànies són constants. Sota aquesta hipòtesi d'homogeneïtat respecte al temps, les taxes de substitució es representen mitjançant les entrades d'una matriu de taxes Q i les matrius de transició $M(t)$ del procés de Markov satisfan $M(t) = Qt$ per a qualsevol $t \geq 0$ i per tant són embeddables. Així doncs, en el context dels processos de Markov, el problema d'embedding consisteix a decidir si unes certes probabilitats de substitució poden sorgir d'un procés homogeni en temps continu.

El problema d'embedding per a matrius 2×2 va ser resolt per Kingman (vegeu [Kin62]). Tal i com s'explica en aquest article, una matriu 2×2 és embeddable si, i només si, té determinant positiu. Per tant, en aquest cas es pot decidir fàcilment si una matriu de Markov és embeddable. Tot i això, en el mateix article l'autor expressa els seus dubtes respecte a la possibilitat d'obtenir una solució senzilla per a casos més grans i fins i tot posa en dubte que es pugui obtenir una solució explícita per al problema d'embedding. Tal i com s'ha vist més tard, aquestes afirmacions no anaven del tot desencaminades. El problema d'embedding també està resolt per a matrius 3×3, però en aquest cas la solució és molt més complicada. De fet, la solució està dividida en diferents casos segons la forma de Jordan de la matriu de Markov i s'han necessitat gairebé quaranta anys per a resoldre explícitament tots els casos (vegeu les contribucions més rellevants: [Cut73, Joh74, Car95, CC11]). Tot i que existeixen alguns resultats per a casos particulars de matrius $n \times n$, fins ara no ha estat possible resoldre el problema d'embedding per a matrius 4×4 o més grans.

Un problema relacionat amb el d'embedding és el d'identificabilitat de taxes. Mentre que en el problema d'embedding es pregunta si una matriu donada té un generador de Markov, en el *problema d'identificabilitat* es pressuposa l'existència de generadors i se'n qüestiona la unicitat. Així doncs, diem que una matriu embeddable té *taxes identificables* si té un únic generador de Markov. Es coneixen múltiples exemples de matrius embeddables sense identificabilitat de taxes (vegeu, per exemple, [Spe67, SS76, Dav10]).

Objectiu 2 (Identificabilitat de taxes)**:** Caracteritzar les matrius embeddables que tenen un únic generador de Markov.

L'estudi del problema d'identificabilitat de taxes també té conseqüències en el problema d'embedding. Per exemple, se sap de vàries condicions que garanteixen que el logaritme principal d'una matriu de Markov n'és el seu únic logaritme real o l'únic logaritme amb files que sumen zero (vegeune alguns exemples a [Cul66, Cut72, SS76]). Com que els generadors de Markov han de ser logaritmes de la matriu de Markov per definició, això dóna lloc a solucions parcials del problema d'embedding que consisteixen a comprovar si el logaritme principal de la matriu de Markov és una matriu de taxes o no. De fet, tots els exemples de matrius embeddables amb valors propis diferents (fins i tot els que no tenen taxes identificables) que coneixíem abans de la feina presentada en aquest llibre, satisfan que el seu logaritme principal és una matriu de taxes.

Objectiu 3: Estudiar si l'embeddabilitat d'una matriu de Markov (*amb valors propis simples*) està determinada pel seu logaritme principal.

Tot i que el problema d'embedding és essencialment teòric, s'ha estudiat detalladament en moltes àrees aplicades degut a les seves implicacions en modelització. Per exemple, en ciències econòmiques [IRW01, GMZ86], en ciències socials [SS76] o en biologia evolutiva [VYP+13, Jia16, KK17, BS20]. Originalment, el nostre interès pel problema ve motivat per la filogenètica (l'estudi de les relacions evolutives), on el problema d'embedding està relacionat amb qüestions fonamentals respecte a la definició i consistència dels models de substitució de nucleòtids. Aquests models sovint descriuen la substitució de nucleòtids en una cadena d'ADN al llarg del temps mitjançant un procés de Markov amb quatre estats, un per a cadascun dels different nucleòtids (adenina, guanina, citosina i timina).

Tradicionalment, els models de substitució de nucleòtids consideren processos de Markov homogenis i en temps continu (vegeu, per exemple, [JC69, Kim81, Fel81, Tav86]). Encara que els processos evolutius reals no són homogenis en general (e.g. [HPCD05]), qualsevol procés de substitució en temps continu es pot aproximar mitjançant la concatenació de processos homogenis curts. En aquest cas, la matriu de transició per al procés sencer s'obté multiplicant les matrius de transició corresponents als processos concatenats (que són embeddables). Si la matriu resultant també és embeddable, aleshores el procés original es pot modelar com si fos homogeni. Tot i això, el producte de matrius embeddables no té per què ser una matriu embeddable i per tant és necessari tenir en compte el problema d'embedding en aquest context, encara que les matrius de transició dels models en temps continu siguin embeddables per construcció.

Alternativament, es pot evitar considerar el temps i simplement utilitzar una matriu de Markov per descriure el procés de substitució complet. Aquest enfocament és més general que no pas el dels processos homogenis en temps continu perquè considera *totes* les matrius de Markov, independentment de si són embeddables o no. D'altra banda, aquesta generalitat no té per què ser completament positiva, ja que algunes de les matrius afegides descriuen processos evolutius que es podrien considerar poc realistes (per exemple, les matrius de permutació). Quan no es treballa en temps continu, els paràmetres del model són les probabilitats de substitució entre nucleòtids en lloc de les taxes instantànies de mutació. El fet de treballar amb aquestes probabilitats permet l'ús de tècniques típiques de la geometria algebraica i de l'àlgebra commutativa per a estudiar les propietats geomètriques del model (vegeu [SS05, AR07, AR08, DK09]). Al seu torn, aquests estudis han permès trobar diversos mètodes algebraics per a reconstruir la història evolutiva d'un conjunt d'espècies donades sense necessitat d'estimar els paràmetres de substitució (vegeu, per exemple, [Eri05, CFS07, RH12, CK14, AKR17]). Cal remarcar que aquests mètodes de reconstrucció filogenètica també es poden utilitzar en processos de substitució homogenis en temps continu. De fet, existeixen mètodes de reconstrucció amb una base algebraica que s'han definit explícitament per a models homogenis en temps continu (vegeu [SCJJ08, HJS13]).

La connexió entre aquests dos tipus de models de substitució (en temps continu o sense considerar el temps) està íntimament lligada al problema d'embedding, ja que les matrius de Markov són descartades o potencialment considerades segons l'enfocament.

Objectiu 4: Quantificar la proporció de matrius de transició 4×4 que són consistents amb l'enfocament dels models de substitució de nucleòtids homogenis i en temps continu (i.e., que són embeddables).

Segons el context, les hipòtesis dels diferents models de substitució de nucleòtids s'expressen com a restriccions en termes de les taxes instantànies de mutació o en termes de les probabilitats de substitucions. Aquestes restriccions solen estar motivades per observacions de les freqüències de substitucions entre nucleòtids (vegeu per exemple els models de Kimura [Kim80, Kim81]) o per conveniència matemàtica (com és el cas del model de Felsenstein [Fel04] o del model GTR [Tav86]). Sembla natural preguntar-se quan una matriu de transició subjecta a les restriccions d'un cert model admet un generador de Markov que satisfaci les mateixes restriccions. Quan això passa, diem que la matriu de transició és *model-embeddable*.

Objectiu 5: Donat un model de substitució de nucleòtids, quantificar-ne la proporció de matrius de transició embeddable i model-embeddable.

B.2 RESULTATS PRINCIPALS

El capítol 1 és introductori. Aquí presentem les definicions i els resultats ja coneguts que necessitarem posteriorment i posem en context el problema d'embedding de manera detallada. També introduïm dos resultats fonamentals per a les nostres contribucions: la descripció de tots els logaritmes d'una matriu qualsevol i la caracterització de les matrius que tenen algun logaritme real (vegeu [Gan59] i [Cul66], respectivament). A l'última secció, ens centrem en els models de substitució de nucleòtids i en l'impacte que hi té el problema d'embedding. A més a més justifiquem que totes les matrius embeddables són biològicament significatives (vegeu la remarca 1.4.13).

Al capítol 2 estudiem els problemes d'embedding i d'identificabilitat de taxes per a matrius de Markov de qualsevol mida (Objectius 1 i 2). En primer lloc, millorem les cotes existents per als valors propis de les matrius de taxes. Això ens permet trobar una condició suficient per a garantir l'embeddabilitat d'una matriu de Markov $n \times n$ amb una hipòtesi més relaxada que en altres resultats semblants (cf. [Cut73, IRW01]).

Teorema 1 (Teorema 2.2.5). *Sigui M una matriu de Markov $n \times n$ i diagonalitzable. Per a tot valor propi $z \in \sigma(M)$ definim*

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

Si per a tot valor propi amb part imaginària no nul·la o amb multiplicitat major que 1 es satisfà que $\beta_n(z) \leq \pi$, aleshores M és embeddable si, i només si, el seu logaritme principal és una matriu de taxes. En aquest cas, les taxes d'M són identificables (i vénen donades per $\mathrm{Log}(M)$).

A més a més d'aquesta solució particular del problema d'embedding (i del problema d'identificabilitat de taxes), també donem el següent criteri per a comprovar si una matriu de Markov $n \times n$ amb valors propis diferents (reals o no) és embeddable:

Teorema 2 (Theorem 2.3.3). *Sigui M una matriu de Markov amb valors propis diferents dos a dos. Donada una descomposició d'M en valors propis qualsevol:*

$$M = P\,\mathrm{diag}\big(1, \lambda_1, \ldots, \lambda_t, \mu_1, \overline{\mu_1}, \ldots, \mu_s, \overline{\mu_s}\big)\,P^{-1},$$

amb $P \in GL_n(\mathbb{C})$, $\lambda_i \in (0,1)$ per $i = 1, \ldots, t$ i $\mu_j \in \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$ per $j = 1, \ldots, s$; tenim que M és embeddable si i només si

$$P\,\mathrm{diag}\Big(0, \log(\lambda_1), \ldots, \log(\lambda_t), \log_{k_1}(\mu_1), \overline{\log_{k_1}(\mu_1)}, \ldots, \log_{k_s}(\mu_s), \overline{\log_{k_s}(\mu_s)}\Big)\,P^{-1}$$

és una matriu de taxes per alguns valors $k_1, \ldots, k_s \in \mathbb{Z}^s$ tals que

$$\left\lceil \tfrac{-\mathrm{Arg}(\mu_j) - \beta_n(\mu_j)}{2\pi} \right\rceil \leq k_j \leq \left\lfloor \tfrac{-\mathrm{Arg}(\mu_j) + \beta_n(\mu_j)}{2\pi} \right\rfloor.$$

Basant-nos en aquest resultat, aconseguim un algoritme que permet trobar tots els generadors de Markov de qualsevol matriu de Markov diagonalitzable i sense valors propis repetits (Algoritme 2.3.5). Aquest algoritme resol tant el problema d'embedding com el d'identificabilitat de taxes per a un subconjunt dens de matrius de Markov $n \times n$ per a tot $n \in \mathbb{N}$.

Al capítol 3 resolem completament el problema d'embedding per a matrius 4×4. Com en el cas 3×3, la nostra solució es divideix en diversos casos segons la forma de Jordan de la matriu de Markov donada (vegeu la taula 3.2). El cas de matrius de Markov amb valors propis diferents dos a dos es resol mitjançant l'especialització dels resultats del capítol anterior. Aquest cop, obtenim un criteri explícit tant per a l'embeddabilitat com per a la identificabilitat de taxes.

Teorema 3 (Teorema 3.2.1)**.** *Sigui* $M = P\mathrm{diag}(1, \lambda_1, \lambda_2, \lambda_3)P^{-1}$ *una matriu de Markov* 4×4 *amb valors propis* $\lambda_1 \in \mathbb{R}_{>0}$*,* $\lambda_2 \in \mathbb{C}$*,* $\lambda_3 \in \mathbb{C}$ *diferents dos a dos. Si* $\lambda_2, \lambda_3 \notin \mathbb{R}$*, definim* $V = P\ \mathrm{diag}(0, 0, 2\pi i, -2\pi i)\ P^{-1}$ *i*

$$\mathcal{L} := \max_{(i,j):\ i\neq j,\ V_{i,j}>0} \left\lceil -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rceil, \quad \mathcal{U} := \min_{(i,j):\ i\neq j,\ V_{i,j}<0} \left\lfloor -\frac{\mathrm{Log}(M)_{i,j}}{V_{i,j}} \right\rfloor.$$

En cas contrari, prenem $\mathcal{L} = \mathcal{U} = 0$ *i fixem que* V *sigui la matriu zero. Donada la matriu* V *definim*

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

Aleshores M *és embeddable si i només si* $\mathcal{N} = \emptyset$*,* $\mathcal{L} \leq \mathcal{U}$ *i* $\lambda_i \notin \mathbb{R}_{\leq 0}$ *per* $i = 1, 2, 3$*. En aquest cas, els generadors de Markov per a* M *són les matrius* $\mathrm{Log}(M) + kV$ *amb* $k \in [\mathcal{L}, \mathcal{U}]$*.*

També donem un algoritme per comprovar l'embeddabilitat de les matrius de Markov 4×4 amb un valor propi amb multiplicitat 2 (Algoritme 3.2.3) i un algoritme per a comprovar l'embeddabilitat de la resta de matrius (Algorithm 3.2.2). Utilitzant aquest últim algoritme en un conjunt de matrius de Markov 4×4 (amb valors propis diferents) generat aleatòriament d'acord amb la distribució uniforme, podem estimar la proporció de matrius embeddables dins del conjunt de matrius de Markov 4×4 (Objectiu 4). D'acord amb els resultats obtinguts, només un 0.05% de les matrius de Markov 4×4 és embeddable (vegeu la taula 3.1).

Al capítol 4 resolem el problema d'embedding per al model de substitució de nucleòtids Kimura 3-paràmetres [Kim81] i per als seus submodels, el model Kimura 2-paràmetres [Kim80] i el model de Jukes-Cantor [JC69].

Teorema 4 (vegeu la proposició 3.1.14 i els corol·laris 4.2.1 i 4.2.6)**.** *Sigui* M *una matriu de Markov corresponent al model de Kimura 3-paràmetres* *amb valors propis* $1, \lambda, \mu, \gamma$. *Si tots els valors propis d'M són simples, les següents afirmacions són equivalents:*

i) M és embeddable.

ii) M és model-embeddable.

iii) El logaritme principal d'M és una matriu de taxes.

iv) Els valors propis d'M són estrictament positius i satisfan

$$\lambda \geq \mu\gamma, \qquad \mu \geq \lambda\gamma, \qquad \gamma \geq \lambda\mu.$$

Aquest resultat mostra que la conjectura estudiada a l'objectiu 3 és certa quan ens restringim al model Kimura 3-paràmetres. En aquest capítol també estudiem detalladament aquelles matrius de Markov dins del model que tenen un valor propi amb multiplicitat 2. De fet, veurem que es pot considerar sense pèrdua de generalitat que pertanyen també al model Kimura 2-paràmetres. Així doncs, el següent resultat dóna un criteri per a la embeddabilitat i la identificabilitat de taxes de les matrius de transició del model Kimura 3-paràmetres que tenen algun valor propi amb multiplicitat 2.

Teorema 5 (Teorema 4.3.8)**.** *Donada una matriu de transició del model Kimura 2-paràmetres* $M = \begin{pmatrix} a & b & c & c \\ b & a & c & c \\ c & c & a & b \\ c & c & b & a \end{pmatrix}$ *tal que* $b \neq c$, *tenim:*

a) Si $c = 0.5 - b$, *M no és embeddable.*

b) Si $c < 0.5 - b$, *aleshores M és embeddable si i només si* $c \leq \sqrt{b} - b$. *En aquest cas,*

i) Si $c < \frac{1-e^{-4\pi}}{4}$, *aleshores les taxes d'M són identificables.*

ii) Si $c = \frac{1-e^{-4\pi}}{4}$, *aleshores M té exactament* 3 *generadors de Markov.*

iii) Si $c > \frac{1-e^{-4\pi}}{4}$, *aleshores M té una quantitat no numerable de generadors de Markov.*

c) Si $c > 0.5 - b$*, aleshores* M *és embeddable si i només si* $\frac{1-e^{-2\pi}}{4} \leq c \leq \sqrt{b} - b$*. En aquest cas, les taxes d'M no són identificables, és més:*

i) Si $c = \frac{1-e^{-2\pi}}{4}$*, aleshores* M *té exactament* 2 *generadors de Markov*

ii) Si $c > \frac{1-e^{-2\pi}}{4}$*, aleshores* M *té una quantitat no numerable de generadors de Markov.*

A diferència del model Kimura 3-paràmetres, veiem que les matrius del model Kimura 2-paràmetres que són embeddables poden no tenir taxes identificables. No només això, sinó que algunes matrius embeddables dins del model Kimura 2-paràmetres no són model-embeddables, la qual cosa sembla ser inconsistent amb l'enfocament original d'aquests models mitjançant taxes de mutació, en el qual les restriccions en les taxes s'inferien a partir de les probabilitats de substitució.

Concloem el capítol calculant la proporció de matrius embeddables i model-embedabbles dins dels models Kimura 3-paràmetres, Kimura 2-paràmetres i Jukes-Cantor (Objectiu 5). Veurem que només el 9.375% de les matrius de transició corresponents al model de Kimura 3-paràmetres són embeddables. Per al model Kimura 2-paràmetres la proporció de matrius embeddables és lleugerament superior al 33% mentre que el model de Jukes-Cantor té un 75% de matrius de transició embeddables.

Al capítol 5 hi estudiem el model strand-symetric (vegeu [YP04, CS05]). Sota la hipòtesis de valors propis simples, veiem que la embeddabilitat i la model-embeddabilitat són equivalents per a aquest model (Proposition 5.1.2) i donem un condició necessària per tal que se satisfacin.

Teorema 6 (Teorema 5.1.8)**.** *Sigui* M *una matriu de transició pertanyent al model strand-symmetric i amb valors propis simples. Si* M *és embeddable, aleshores al menys una de les següents afirmacions és certa:*

i) $\text{Log}(M)$ *és una matriu de taxes.*

ii) $\text{Log}(M)$ *no té cap entrada igual a zero i té exactament dues entrades negatives fora de la diagonal, les quals estan a l'anti-diagonal de la matriu.*

Tot i que no donem un criteri explícit per a l'embeddabilitat de les matrius de transició del model strand-symmetric, podem estimar-ne la proporció aplicant l'algoritme 3.2.2 a una mostra aleatòria de matrius generada uniformement d'acord amb el model. Els resultats obtinguts mostren que aproximadament l'1.75% de matrius de transició del model strand-symmetric són embeddables. Acabem el capítol construint una família d'exemples de matrius de Markov dins d'aquest model que mostren que la conjectura estudiada a l'objectiu 3 pot ser falsa (vegeu els exemples 5.2.4 i 5.2.5). A més a més, pertorbem aquests exemples i demostrem que és *genèricament* fals que l'embeddabilitat d'una matriu de Markov 4×4 es pugui determinar únicament a partir del seu logaritme principal.

Teorema 7 (vegeu el teorema 5.3.1)**.** *Existeix un subconjunt obert de matrius de Markov* 4×4 *amb mesura positiva (en la norma euclidiana) format per matrius que són embeddables i que el seu logaritme principal no és una matriu de taxes.*

Concloem aquest resum fent una síntesi dels resultats obtinguts per a l'objectiu 5 respecte als models de substitució de nucleòtids considerats al llarg dels capítols 3, 4 i 5. Excepte per al model Kimura 2-paràmetres, els conjunts de matrius embeddable i model-embeddable dins d'aquests models són idèntics. Observem que com més simple és el model, més gran és la proporció de matrius embeddable.

Model	**Proporció de matrius embeddables**
General Markov	0.00057
Strand symmetric	0.0175
Kimura 3-paràmetres	0.09375
Kimura 2-paràmetres	0.33336
Jukes-Cantor	0.75