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Some geometric properties of stochastic matrices

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Abstract. We study geometric aspects of transition matrices of discrete-time Markov chains. More precisely, we study the connected component of the set of stochastic matrices with positive determinant at the identity. Using the machinery of Lie groups we explore the connection between stochastic matrices and transition rate matrices.

Palavras-chave. Discrete-time Markov chains, Continuous-time Markov chains, Stochastic matrices, Lie group, Lie algebra.

1 Introduction

When we study discrete-time and continuous-time Markov chains we are interested in the following question: Is there any way to generate a discrete time Markov chain by means of a transition rate matrix? In [6] Jeremy G. Summer studied the algebraic properties of the Lie group \mathcal{G} of stochastic matrices of order 2 and its tangent space $T_1(\mathcal{G})$ which is a Lie algebra. He showed that the following decomposition holds

$$\mathcal{G}^0 = \bigcup_{t \in \mathbb{R}} e^{Qt} \mathcal{H}, \quad (1)$$

where \mathcal{G}^0 is the connected component at the identity of the set of stochastic matrices with positive determinant, \mathcal{H} a normal subgroup of \mathcal{G}^0 and Q is a transition rate matrix. Thus, for stochastic matrices of order 2 there is a positive answer to the question above.

Our main result is a generalization of the result obtained in [6] for stochastic matrices of any size.

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2 Stochastic Matrices

Discrete time Markov chains $(X_n, n \in \mathbb{N})$ and continuous time Markov chains $(X_t, t \geq 0)$ with countable state space Ω can be characterized by its transition matrix $M = (M_{ij})_{i,j \in \Omega}$ and by means of its transition rate matrix $L = (L_{ij})_{i,j \in \Omega}$, respectively. These matrices must satisfy the following conditions:

1. $M_{ij} \geq 0$ for all $i, j \in \Omega$ and $\sum_j M_{ij} = 1$ for all $i \in \Omega$. Such matrices are called *transition matrices* or *stochastic matrices*.
2. $L_{ii} \leq 0$ for all $i \in \Omega$ and $L_{ij} \geq 0$ for all elements $i \neq j$ in the state space. In addition, equality $\sum_j L_{ij} = 0$ must be valid for all $i, j \in \Omega$. Matrices that satisfy these conditions are called *transition rate matrices* or *L-matrices*.

In this work we study a way to generate Markov chains in discrete time by means of L-matrices. When we study the Lie group of matrices given by the stochastic matrices, we note that there is a relation with its tangent space which contains the desired L-matrices. These relations were studied in [6] for the case of square matrices of dimension 2. In this work we generalize this results to stochastic matrices of any size.

2.1 The group of stochastic matrices and its tangent space

Let $\mathbf{1} = (1, 1, \dots, 1)$ be a vector with n coordinates. We say that a real matrix $A = (a_{ij})_{n \times n}$ is stochastic if the condition below is verified

$$A \cdot \mathbf{1} = \mathbf{1} \quad \text{e} \quad 0 \leq a_{ij} \leq 1, \forall i, j \in \{1, 2, \dots, n\}. \quad (2)$$

Now we define the following set:

$$\mathcal{G}_n = \{A \in GL_n(\mathbb{R}); A \cdot \mathbf{1} = \mathbf{1}\}. \quad (3)$$

The set \mathcal{G}_n defined in this way is a subgroup of the general linear group. We call \mathcal{G}_n the stochastic matrix group. Indeed, \mathcal{G}_n is a Lie group. To show our claim it suffices to show that \mathcal{G}_n is a closed subset of $GL_n(\mathbb{R})$. For this purpose, consider the function $\phi : GL_n(\mathbb{R}) \rightarrow \mathbb{R}^n$ given by $A \mapsto A \cdot \mathbf{1}$. Let $A, B \in GL_n(\mathbb{R})$. Then, ϕ satisfies

$$\|\phi(A) - \phi(B)\| = \|(A - B) \cdot \mathbf{1}\| \leq \sqrt{n} \cdot \|A - B\|. \quad (4)$$

It follows from (4) that ϕ is Lipschitz and hence it is a continuous function. Since $\{\mathbf{1}\}$ is a closed subset of \mathbb{R}^n and ϕ is continuous, we may conclude that \mathcal{G}_n is a closed subset of the general linear group. This proves our claim.

Now we study the tangent space of the Lie group \mathcal{G}_n . Given a differentiable path $A : [0, 1] \rightarrow \mathcal{G}_n$, with $A(0) = I_n$, and using the constraint $A(t) \cdot \mathbf{1} = \mathbf{1}$ for all $t \in [0, 1]$, we get $A'(t) \cdot \mathbf{1} = \mathbf{0}$. Therefore, we conclude that $A'(0) \cdot \mathbf{1} = \mathbf{0}$ and $T_1(\mathcal{G}_n) \subseteq \{X \in GL_n(\mathbb{R}); X \cdot \mathbf{1} = \mathbf{0}\}$. Given a matrix A with eigenvalue λ and eigenvector v , we have $e^{tA}v = e^{t\lambda}v$, for any $t \in \mathbb{R}$. In particular for any matrix $A \in \{X \in GL_n(\mathbb{R}); X \cdot \mathbf{1} = \mathbf{0}\}$ (with eigenvector $\mathbf{1}$ and eigenvalue 0), $e^{tA}\mathbf{1} = e^{t0}\mathbf{1} = \mathbf{1}$. Since $e^{tA} \in \mathcal{G}_n$ for any $t \in [0, 1]$, the

function $f(t) = e^{tA}$ have the following properties: (i) $f(0) = \mathbf{I}_n$ and (ii) $f'(0) = A \in T_1(\mathcal{G}_n)$. Therefore, we conclude that $\{X \in GL_n(\mathbb{R}); X \cdot \mathbf{1} = \mathbf{0}\} \subseteq T_1(\mathcal{G}_n)$ and we obtain the desired equality $T_1(\mathcal{G}_n) = \{X \in GL_n(\mathbb{R}); X \cdot \mathbf{1} = \mathbf{0}\}$.

Since $X = (x_{ij}) \in T_1(\mathcal{G}_n)$, $\sum_{j=1}^n x_{ij} = 0, \forall i \in \{1, 2, \dots, n\}$. Therefore, using elementary matrices E_{ij} , we get

$$X = \sum_{\substack{i \in \{1, \dots, n\} \\ j \in \{1, \dots, n-1\}}} x_{ij} \cdot (E_{ij} - E_{in}). \tag{5}$$

Hence, $\dim_{\mathbb{R}} T_1(\mathcal{G}_n) = n(n - 1)$. In this section we show how the connected component at the identity of \mathcal{G}_n , denoted by \mathcal{G}_n^0 , is related to transition rate matrices of a continuous time Markov chains. For this purpose, we use the following result.

Proposition 2.1. *The set of stochastic matrices with positive determinant is path-connected.*

The proof of this proposition is given in the end of the section. In possession of this result one immediately obtain the following corollary.

Corollary 2.1. *The connected component \mathcal{G}_n^0 of the group of stochastic matrices at the identity is given by the set of stochastic positive-determinant matrices, i.e.*

$$\mathcal{G}_n^0 = \{X \in \mathcal{G}_n; \det(X) > 0\}. \tag{6}$$

Proof. It is well known, see [3] for instance, that the connected component of the general linear group is given by the set of matrices with positive determinant; therefore $\mathcal{G}_n^0 \subseteq \{X \in \mathcal{G}_n; \det(X) > 0\}$. Conversely, it follows from the proposition 2.1 that the set of stochastic matrices with positive determinant is path-connected which finishes the proof. \square

In possession of this result one immediately obtain the following theorem.

Theorem 2.1. *Let \mathcal{G}_n be the group of stochastic matrices and \mathcal{G}_n^0 the connected component at the identity. Let $\mathcal{H} := \{A \in \mathcal{G}_n : \det(A) = 1\}$. Then, there exists a L -matrix Q_0 such that the decomposition $\mathcal{G}_n^0 = \bigcup_{t \in \mathbb{R}} e^{Q_0 t} \mathcal{H}$ is valid.*

In the proof of the theorem above we follow the approach introduced in [6].

Proof. Let $\mathbb{R}_{>0}$ be the multiplicative group of nonnegative real numbers with identity 1. There exists a group homomorphism ψ between \mathcal{G}_n^0 and $\mathbb{R}_{>0}$ given by $X \mapsto \det(X)$. It easily follows that $\mathcal{G}_n^0 / \ker(\psi) \cong \text{Im}(\psi)$. Observe that \mathcal{H} is a subnormal group of \mathcal{G}_n^0 . Since $\ker(\psi) = \mathcal{H}$ and, by corollary 2.1, $\text{Im}(\psi) = \mathbb{R}_{>0}$, it follows that $\mathcal{G}_n^0 / \mathcal{H} \cong \mathbb{R}_{>0}$. Therefore we can safely write the connected component as $\mathcal{G}_n^0 = \bigcup_{Q \in \mathcal{G}_n^0} Q\mathcal{H}$. Finally, fix a matrix $Q_0 \in T_1(\mathcal{G}_n)$ with nonzero trace. We already know that $e^{Q_0} \in \mathcal{G}_n$ and that $\det(e^{Q_0}) = e^{\text{tr}(Q_0)} > 0$, i.e. $e^{Q_0} \in \mathcal{G}_n^0$. In addition, given two matrices $M, P \in \mathcal{G}_n^0$, we know that $M\mathcal{H} = P\mathcal{H} \iff \det(M) = \det(P)$. Consequently, given a any matrix $Q \in \mathcal{G}_n^0$ and choosing $t_0 = \ln(\det(Q)) / \text{tr}(Q_0)$, we get that $\det(e^{t_0 Q_0}) = e^{t_0 \text{tr}(Q_0)} = \det(Q)$, i.e., $Q\mathcal{H} = (t_0 Q_0)\mathcal{H}$. Therefore $\mathcal{G}_n^0 = \bigcup_{t \in \mathbb{R}} e^{Q_0 t} \mathcal{H}$. This finishes the proof. \square

Corollary 2.2. *For any matrix $M \in \mathcal{G}_n$ with positive determinant, there exists $t_0 > 0$, a matrix $P \in \mathcal{G}_n^0$ of determinant one and a L-matrix Q_0 such that*

$$M = e^{Q_0 \cdot t_0} e^P. \tag{7}$$

2.2 Example

Now we use Corollary 2.2 above in order to provide a numerical example of our results. Indeed, we provide an example of a transition matrix M using equality (7). Let P be matrix whose trace is not zero and such that the sum of its entries in each row is zero and let Q_0 be a transition rate matrix

$$Q_0 = \frac{1}{3} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \end{pmatrix}, \quad P = \begin{pmatrix} 0,1070 & 0,3447 & -0,4517 \\ 0,0462 & 0,1351 & -0,1813 \\ 0,9554 & -0,7133 & -0,2421 \end{pmatrix}.$$

Let $t_0 = 4,3329$. It follows from (7) that

$$M = \begin{pmatrix} 0,4415 & 0,5543 & 0,0042 \\ 0,3771 & 0,4091 & 0,2138 \\ 0,4257 & 0,3147 & 0,2596 \end{pmatrix}$$

is a transition matrix.

2.3 Proof of Proposition 2.1

Let \mathbf{I}_k denotes the identity matrix of order k , let $\mathbf{0}_{k \times l}$ denotes the zero matrix with k rows and l columns and $\mathbf{P}_{2 \times 2}^{(1)}, \dots, \mathbf{P}_{2 \times 2}^{(n)}$ denotes 2×2 stochastic matrices. Denote by $\mathbf{W}^{(i)} \in GL_{n+1}(\mathbb{R})$ a block matrix of the following kind

$$\mathbf{W}^{(i)} = \begin{pmatrix} \mathbf{I}_{(i-1) \times (i-1)} & \mathbf{0}_{(i-1) \times 2} & \mathbf{0}_{(i-1) \times (n-i)} \\ \mathbf{0}_{2 \times (i-1)} & \mathbf{P}_{2 \times 2}^{(i)} & \mathbf{0}_{2 \times (n-i)} \\ \mathbf{0}_{(n-i) \times (i-1)} & \mathbf{0}_{(n-i) \times 2} & \mathbf{I}_{(n-i) \times (n-i)} \end{pmatrix}.$$

We say that matrix \mathbf{X} is of type $\mathbf{W}^{(i)}$ for $i \in \{1, \dots, n\}$ if $\mathbf{X} = \mathbf{W}^{(i)}$. Before proving Proposition 2.1, we will prove the following lemma.

Lemma 2.1. *Let $\mathbf{Q} \in \mathcal{G}_{(n+1)}^0$ and let $n \geq 2$. Then, there exists a finite sequence of matrices with positive determinant $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_m$ such that*

$$\mathbf{Q} \cdot \mathbf{X}_1 \cdot \mathbf{X}_2 \cdots \mathbf{X}_m = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ y_{2,1} & y_{2,2} & \cdots & y_{2,n+1} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n+1,1} & y_{n+1,2} & \cdots & y_{n+1,n+1} \end{pmatrix}.$$

Moreover, the matrices $\mathbf{X}_i, i \in \{1, \dots, m\}$ are of type $\mathbf{X}_i = \mathbf{W}^{(j)}$ for some $j \in \{1, \dots, n\}$.

Proof. Let $\mathbf{Q} \in \mathcal{G}_{(n+1)}$ ($n \geq 2$) with positive determinant be given. The first step of the proof consist in showing that there exists two matrices $\mathbf{X}_1, \mathbf{X}_2$ such that

$$\mathbf{Q} \cdot \mathbf{X}_1 \cdot \mathbf{X}_2 = \mathbf{Q}^{(1)}, \tag{8}$$

where $\mathbf{Q}^{(1)}$ is a square matrix of order $(n + 1)$ given by

$$\mathbf{Q}^{(1)} = \begin{pmatrix} Q_{1,1}^{(1)} & Q_{1,2}^{(1)} & \cdots & Q_{1,n}^{(1)} & 0 \\ Q_{2,1}^{(1)} & Q_{2,2}^{(1)} & \cdots & Q_{2,n+1}^{(1)} & Q_{2,n+1}^{(1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ Q_{n+1,1}^{(1)} & Q_{n+1,2}^{(1)} & \cdots & Q_{n+1,n+1}^{(1)} & Q_{n+1,n+1}^{(1)} \end{pmatrix}.$$

In order to show this equality we must divide its proof into three parts. Indeed, we shall consider the following cases: (i) $Q_{1,n} + Q_{1,n+1} > 0$, (ii) $Q_{1,n} + Q_{1,n+1} < 0$ and (iii) $Q_{1,n} + Q_{1,n+1} = 0$.

If $Q_{1,n} + Q_{1,n+1} > 0$, take the matrix \mathbf{X}_1 given by

$$\mathbf{X}_1 = \mathbf{W}^{(n)} = \begin{pmatrix} \mathbf{I}_{(n-1) \times (n-1)} & \mathbf{0}_{(n-1) \times 2} \\ \mathbf{0}_{2 \times (n-1)} & \mathbf{P}_{2 \times 2}^{(n)} \end{pmatrix} \text{ with } \mathbf{P}_{2 \times 2}^{(n)} = \begin{pmatrix} 1 + Q_{1,n+1} & -Q_{1,n+1} \\ 1 - Q_{1,n} & Q_{1,n} \end{pmatrix} \text{ and}$$

$\mathbf{X}_2 = \mathbf{I}_{(n+1) \times (n+1)}$. Thus, $\mathbf{Q} \cdot \mathbf{X}_1 \cdot \mathbf{X}_2 = \mathbf{Q}^{(1)}$ with $\det(\mathbf{X}_1) = Q_{1,n} + Q_{1,n+1} > 0$.

We can continue this process inductively obtaining two sequences of matrices $\mathbf{Q}^{(1)}, \mathbf{Q}^{(2)}, \dots, \mathbf{Q}^{(n-1)}$ and $X_1, \dots, X_{2(n-1)+1}$ such that

$$\mathbf{Q}^{(n-1)} = \begin{pmatrix} Q_{1,1}^{(n-1)} & Q_{1,2}^{(n-1)} & 0 & \cdots & 0 & 0 & 0 \\ Q_{2,1}^{(n-1)} & Q_{2,2}^{(n-1)} & Q_{2,3}^{(n-1)} & \cdots & Q_{2,n-1}^{(n-1)} & Q_{2,n}^{(n-1)} & Q_{2,n+1}^{(n-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ Q_{n+1,1}^{(n-1)} & Q_{n+1,2}^{(n-1)} & Q_{2,3}^{(n-1)} & \cdots & Q_{n+1,n-1}^{(n-1)} & Q_{n+1,n}^{(n-1)} & Q_{n+1,n+1}^{(n-1)} \end{pmatrix}$$

and $\mathbf{Q} \cdot \mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{(n-1) \cdot 2+1} = \mathbf{Q}^{(n)}$ where

$$\mathbf{Q}^{(n)} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ Q_{2,1}^{(n)} & Q_{2,2}^{(n)} & Q_{2,3}^{(n)} & \cdots & Q_{2,n-1}^{(n)} & Q_{2,n}^{(n)} & Q_{2,n+1}^{(n)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ Q_{n+1,1}^{(n)} & Q_{n+1,2}^{(n)} & Q_{2,3}^{(n)} & \cdots & Q_{n+1,n-1}^{(n)} & Q_{n+1,n}^{(n)} & Q_{n+1,n+1}^{(n)} \end{pmatrix}.$$

It follows from the construction above that the matrices $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{(n-1) \cdot 2+1}$ have positive determinant and are of type $\mathbf{W}^{(i)}$. This finishes the proof of case (i). The proof of cases (ii) and (iii) is similar and it is left as exercise for the reader. \square

Using the previous lemma we prove the following proposition which is one of the most important result of the work.

Proposition 2.2. *The set of stochastic matrices with positive determinant is path-connected.*

Proof. The proof is by induction on the size of the stochastic matrix. If $n = 2$, the result was proved in [6]. We assume that the result is valid for a given n and will show that the result holds for $n + 1$.

Let $\mathbf{Q} \in \mathcal{G}_{n+1}$ with positive determinant. It follows from the lemma above that there exists a finite sequence of matrices with positive determinant $\mathbf{X}_1, \dots, \mathbf{X}_m$ such that $\mathbf{Q} \cdot \mathbf{X}_m \cdot \mathbf{X}_{m-1} \cdots \mathbf{X}_1 = \mathbf{Q}'$, where $\mathbf{Q}'_{11} = 1$ and $\mathbf{Q}'_{i1} = 0$ for $i \neq 1$.

Applying elementary operations on \mathbf{Q}' we obtain a new matrix $\tilde{\mathbf{Q}}$ such that $\tilde{\mathbf{Q}}_{i,1} < 1$ for any $i = 2, 3, \dots, n + 1$.

Let \mathbf{P} be the diagonal matrix given by

$$\mathbf{P} = (P_{ij}) \text{ with } P_{ij} = \begin{cases} 1 & \text{if } i = j = 1; \\ \sum_{l=2}^{n+1} \tilde{\mathbf{Q}}_{il} & \text{if } i = j \text{ e } i > 1; \\ 0 & \text{in other case.} \end{cases} \quad (9)$$

Note that $P_{ii} > 0$ for any value of i . Thus, \mathbf{P} is invertible and has positive determinant. Let $\mathbf{Z} := \mathbf{P}^{-1}\tilde{\mathbf{Q}}$. Note that we can write the matrix \mathbf{Z} as a matrix of blocks. Now, using that $\mathbf{P}^{-1} \cdot \tilde{\mathbf{Q}} = \mathbf{Z}$ we have that $\tilde{\mathbf{Q}} = (\mathbf{P} \cdot \mathbf{Z})$. Using a procedure analogous to the proof of Lemma 2.1 we obtain a sequence of stochastic matrices with positive determinant $\mathbf{Y}^{(p)}, \mathbf{Y}^{(p-1)}, \dots, \mathbf{Y}^{(1)}, \mathbf{Q}', \mathbf{Y}$ such that $\tilde{\mathbf{Q}} = \mathbf{Y}^{(p)} \cdot \mathbf{Y}^{(p-1)} \dots \mathbf{Y}^{(1)} \cdot \mathbf{Q}' \cdot \mathbf{Y}$. Therefore $\mathbf{Q}' = [\mathbf{Y}^{(p)} \cdot \mathbf{Y}^{(p-1)} \dots \mathbf{Y}^{(1)}]^{-1}(\mathbf{P} \cdot \mathbf{Z})\mathbf{Y}^{-1}$. Finally, since $\mathbf{Q} \cdot \mathbf{X}_m \cdot \mathbf{X}_{m-1} \cdots \mathbf{X}_1 = \mathbf{Q}'$, we may conclude that $\mathbf{Q} = [\mathbf{Y}^{(p)} \cdot \mathbf{Y}^{(p-1)} \dots \mathbf{Y}^{(1)}]^{-1}(\mathbf{P} \cdot \mathbf{Z})\mathbf{Y}^{-1}[\mathbf{X}_m \cdot \mathbf{X}_{m-1} \cdots \mathbf{X}_1]^{-1}$.

We know that

- The matrices $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_m$ are of type $\mathbf{W}^{(j)}$ and have positive determinant. By induction hypothesis, the continuous paths $\mathbf{X}_i(t)$ satisfy $\mathbf{X}_i(0) = \mathbf{I}_{n+1}$ and $\mathbf{X}_i(1) = \mathbf{X}_i$ for $i = 1, 2, \dots, m$ and $t \in [0, 1]$.
- The same claim is valid for the sequence $\mathbf{Y}, \mathbf{Y}^{(1)}, \mathbf{Y}^{(2)}, \dots, \mathbf{Y}^{(p)}$. We get continuous paths $\mathbf{Y}^{(i)}(t)$ and $\mathbf{Y}(t)$ satisfying

$$\begin{aligned} \mathbf{Y}^{(i)}(0) &= \mathbf{I}_{n+1}, & \mathbf{Y}^{(i)}(1) &= \mathbf{Y}^{(i)}, \\ \mathbf{Y}(0) &= \mathbf{I}_{n+1}, & \mathbf{Y}(1) &= \mathbf{Y}, \text{ with } t \in [0, 1]. \end{aligned} \quad (10)$$

- Finally, we study the product \mathbf{PZ} . Consider the continuous function $\mathbf{P}(t)$ given by a diagonal matrix with elements $1, e^{t \cdot \ln(a_2)}, \dots, e^{t \cdot \ln(a_{n+1})}$ with $t \in [0, 1]$. Since \mathbf{Z} is a matrix of blocks and each block admits a continuous path, then the function $(\mathbf{PZ})(t) = \mathbf{P}(t)\mathbf{Z}(t)$ is continuous, stochastic and satisfies $(\mathbf{PZ})(0) = \mathbf{I}_{n+1}$ with $(\mathbf{PZ})(1) = \mathbf{PZ}$.

Therefore, we can conclude that the function

$$\mathbf{Q}(t) = [\mathbf{Y}^{(p)}(t) \cdot \mathbf{Y}^{(p-1)}(t) \cdots \mathbf{Y}^{(1)}(t)]^{-1}(\mathbf{PZ})(t)\mathbf{Y}^{-1}(t)[\mathbf{X}_m(t) \cdot \mathbf{X}_{m-1}(t) \cdots \mathbf{X}_1(t)]^{-1} \quad (11)$$

is continuous, has positive determinant and is a stochastic matrix in its domain. We also have that $\mathbf{Q}(0) = \mathbf{I}_{n+1}$ and $\mathbf{Q}(1) = \mathbf{Q}$. This finishes the proof. \square

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