

UNIVERSITY OF CALGARY

The Application of Lie Theory to Markov Processes

Computation of the Maximum Likelihood Estimator of the Generator of Continuous Time
Markov Processes from a Stopped Random Variable

by

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A PROJECT

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Abstract

Continuous time Markov processes on finite state spaces and Lie theory have individually been highly productive fields of investigation for more than a century. However, the two fields remain ripe for cross pollination. In particular the application of results from Lie theory will yield novel computational methods for estimation problems in continuous time Markov processes on finite state spaces. In this project we derive the minimal Lie algebra that contains the generators of a continuous time Markov process on a finite state space, and then using the guarantees of algebraic and analytic closure construct a Newton-Raphson algorithm for maximum likelihood estimation of the generator of a continuous time Markov process on a finite state space from stopped random variables using Páde approximations for Taylor series expressions of the first and second order derivatives of the exponential map.

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List of Symbols, Abbreviations and Nomenclature

Symbol	Definition
U of C	University of Calgary
A, B, C, \dots	Matrices, except for I which we take as identity
a, b, c, \dots	Constants
$\vec{a}, \vec{b}, \vec{c}, \dots$	Vectors
$\hat{a}, \hat{b}, \hat{c}, \dots$	Unit vectors
$\vec{\mathbb{1}}$	Row sum vector
$\hat{\mathbb{1}}$	Normalized row sum vector
$St(\hat{\mathbb{1}})$	Stochastic Lie group with respect to $\hat{\mathbb{1}}$
$\mathfrak{st}(\hat{\mathbb{1}})$	Stochastic Lie algebra with respect to $\hat{\mathbb{1}}$
$St(\hat{\mathbb{1}}, \hat{\mathbb{1}})$	Doubly stochastic Lie group with respect to $\hat{\mathbb{1}}$
$\mathfrak{st}(\hat{\mathbb{1}}, \hat{\mathbb{1}})$	Doubly stochastic Lie algebra with respect to $\hat{\mathbb{1}}$
$\hat{a} \otimes \hat{b}$	Kronecker product of unit vectors \hat{a} and \hat{b}
$\langle \hat{a}, \hat{b} \rangle$	Inner product of unit vectors \hat{a} and \hat{b}
$\mathbb{P}[\Sigma]$	Probability measure of a measurable set Σ
$\mathbb{I}[\Sigma]$	Indicator function of a measurable set Σ
\mathcal{F}_t	Filtration of sigma algebras with respect to continuous parameter t
X_t	Stochastic process on the filtration \mathcal{F}_t
$\mathbb{E}[X_t]$	Expectation of X_t
$\mathbb{V}ar[X_t]$	Variance of X_t
$\mathbb{C}ov[X_t, Y_t]$	Covariance of X_t and Y_t
$\mathbb{C}or[X_t, Y_t]$	Correlation of X_t and Y_t
$Ad_X A$	Lie group Adjoint operator XAX^{-1}
$ad_X A$	Lie algebra adjoint operator $[X, A]$

$[A, B]$

Commutator bracket $AB - BA$ of matrices A and B

δ_{ij}

Dirac delta operator

Chapter 1

Introduction

1.1 Motivation and Direction

Markov process have a rich and extensive history in the statistical and probability analysis of fields such as the life sciences, operations research, queuing theory communications, natural language, and machine learning. Have modeled syntax of sentences, disease states, cancer survival, epidemiology and demographics, with models such as phase type, birth-death, and hidden State of the art computational methods are focused on hidden Markov Models on a finite state set, and discrete time steps; assuming all transitions are observed but are obscured with noise. This is the focus of the Baum-Welch and Viterbi algorithms, and more recently RUST models. The work presented in this project concerns continuous time Markov processes on a finite state space, where by definition it is not possible to observe all the transitions. Instead what is observed typical is are stopped statistics, such as first hitting times from one state to another. Chapter 2 first establishes the algebraic and analytic closure properties necessary for Chapter 3. Chapter 2 has a secondary role to help develop the physical intuition for the stochastic Lie group necessary to work through the derivatives and approximations of Chapter 3 Chapter 3 derives the the first and second order derivatives of the exponential map and their Padé Approximation. Chapter 4 derives the maximum likelihood estimators from first hitting times Chapter 5 concludes with summarizing remarks and a discussion of the direction for further investigation. Throughout this work we will attempt to conform to a simplified version of Lamport's guide to structuring and presenting proofs.

1.2 Background

1.2.1 Continuous Time Markov Process

1.2.2 Maximum Likelihood Estimation

1.2.3 Lie Theory

1.2.4 Padé Approximation

1.2.5 Newton-Raphson Method

Chapter 2

The Lie Algebra of the Generators of Continuous Time Markov Processes on Finite State Spaces

2.1 Stochastic Matrices

The classical Lie algebras of physics, like the infinitesimal symmetries of the special unitary algebra $\mathfrak{su}(n)$, are defined with respect to invariants of a Banach algebra, such as the matrix invariants of the determinant, trace, or norm. In contrast stochastic matrices are always characterized with respect to a specific unit vector, which we will denote $\hat{\mathbb{1}}$. In the next two sections we provide an explicit construction and characterization of the Lie algebra of stochastic matrices, building on the original the work of ??.

The common approach to stochastic matrices begins with the restriction that the matrices have non-negative entries with respect to the standard orthonormal basis for the vector space on which it acts; namely $\langle \hat{e}_i, A\hat{e}_j \rangle \geq 0$ for all i, j . In addition to allowing for singular matrices this poses an immediate obstacle to the necessary closure with respect to matrix inversion required for matrix groups. As the inverse of a stochastic matrix need not have non-negative entries with respect to the standard orthonormal basis.

For the moment we will set aside the restriction that the entries be non-negative, and instead begin with a generalization of the concept of fixed row sums. We will show this generalization is preserved by matrix inversion, and then develop an orthonormal basis from which specific matrices with non-negative entries, with respect to the basis, can be constructed. In essence tackling the problem from the reverse direction, starting with the more general idea of fixed row sums, then specifying to matrices with non-negative entries with respect to a constructed orthonormal basis.

Definition 1. A matrix A is stochastic with respect to the unit vector $\hat{\mathbb{1}}$ if $A\hat{\mathbb{1}} = \hat{\mathbb{1}}$

In an n dimensional vector space the vector $\vec{1} = \sqrt{n}\hat{1}$ acts as the row sum operator on matrices stochastic with respect to $\hat{1}$. We will make this claim more precise after we dispense with a few more foundational definitions.

Definition 2. Let $St(\hat{1})$ denote the stochastic Lie group of invertible matrices stochastic with respect to $\hat{1}$

It is tempting to view the name stochastic Lie group has a bait and switch, or at least an abuse of the terminology, given we have removed the usual convex polytope of stochastic matrices and replaced it with a group of invertible matrices with a common eigenvector $\hat{1}$. Previous authors have denoted the convex polytope of stochastic matrices as the stochastic semi-group and the group invertible matrices as the pseudo-stochastic Lie group. One could even consider incorporating Markov into the name, in reference to the fact that the transition matrices of a continuous Markov process on a finite state space are by definition invertible and have common eigenvector $\hat{1}$. However the suffix of Lie group in the name connotes both sufficient additional restrictions to make the name distinct, and still allows for an indication of a relationship with the original concept. Of course, this definition immediately necessitates proof of the claim embedded in the definition.

Lemma 1. $St(\hat{1})$ is a Lie group

Proof. We proceed by working mechanistically through the Lie group axioms.

1. The identity element I is in $St(\hat{1})$. Clearly I is invertible and $I\hat{1} = \hat{1}$.
2. If $A, B \in St(\hat{1})$ then $AB \in St(\hat{1})$. This follows from the computation $AB\hat{1} = A\hat{1} = \hat{1}$.
3. If $A \in St(\hat{1})$ then $A^{-1} \in St(\hat{1})$. Recognize that $A\hat{1} = \hat{1}$ implies $\hat{1} = A^{-1}A\hat{1} = A^{-1}\hat{1}$.
4. Associativity follows from $St(\hat{1})$ being a subgroup of $GL(n)$.
5. Finally, that the matrix product $A^{-1}B$ is smooth for all $A, B \in St(\hat{1})$ likewise follows from $St(\hat{1}) < GL(n)$

□

That $St(\hat{\mathbb{1}})$ is a proper matrix Lie group implies that it must be infinitesimal generated by elements of a Lie algebra.

Definition 3. Let $\mathfrak{st}(\hat{\mathbb{1}})$ denote the stochastic Lie algebra of $St(\hat{\mathbb{1}})$

By infinitesimally generated we mean that every element of $St(\hat{\mathbb{1}})$ is a matrix exponential of some element in $\mathfrak{st}(\hat{\mathbb{1}})$. We can fully characterize this algebra as the set of matrices such that their row sums are zero with respect to $\hat{\mathbb{1}}$.

Lemma 2. *The algebra $\mathfrak{st}(\hat{\mathbb{1}})$ is exactly the set of all matrices with $\hat{\mathbb{1}}$ in their kernel.*

Proof. Working through the forward and backward inclusions we have

1. Suppose $A\hat{\mathbb{1}} = 0$ then from the definition of the matrix exponential we have:

$$\begin{aligned}\exp(A)\hat{\mathbb{1}} &= \sum_{n=0}^{\infty} \frac{1}{n!} A^n \hat{\mathbb{1}} \\ &= \hat{\mathbb{1}} + \sum_{n=1}^{\infty} \frac{1}{n!} 0 \\ &= \hat{\mathbb{1}}\end{aligned}$$

Thus $\exp(A) \in St(\hat{\mathbb{1}})$ implying that $A \in \mathfrak{st}(\hat{\mathbb{1}})$

2. Now begin with the reverse assumption, that $A \in \mathfrak{st}(\hat{\mathbb{1}})$. For all $t \in \mathbb{R}$ we have $\exp(tA)\hat{\mathbb{1}} = \hat{\mathbb{1}}$. Differentiation with respect to t and evaluation at $t = 0$ yields

$$\begin{aligned}0 &= \left. \frac{d}{dt} \hat{\mathbb{1}} \right|_{t=0} \\ &= \left. \frac{d}{dt} \exp(tA) \hat{\mathbb{1}} \right|_{t=0} \\ &= \exp(tA) A \hat{\mathbb{1}} \Big|_{t=0} \\ &= A \hat{\mathbb{1}}\end{aligned}$$

□

Over an n dimensional vector space, the condition on a matrix A that $A\hat{\mathbb{1}} = 0$ places n constraints on the n^2 dimensions of A . This leaves $n^2 - n$ free dimensions on $\mathfrak{st}(\hat{\mathbb{1}})$, when considered as a vector

space. This hints that we can construct a generator of $\mathfrak{st}(\hat{\mathbb{1}})$ from order pairs of basis elements \hat{e}_i for the vector space of $\hat{\mathbb{1}}$. To see how this is done we first construct a useful basis for the vector space to which $\hat{\mathbb{1}}$ is a member.

Lemma 3. *There exists an orthonormal basis \hat{e}_i such that $\langle \hat{e}_i, \hat{\mathbb{1}} \rangle = \frac{1}{\sqrt{n}}$ for all i*

Proof. While a basis with the stipulated properties can be constructed through the Gram-Schmidt process, the proof of the existence of such a basis proceeds by induction.

1. For $n = 1$ the desired basis is precisely the trivial set $\{\hat{\mathbb{1}}\}$ which satisfies the condition that $\langle \hat{\mathbb{1}}, \hat{\mathbb{1}} \rangle = 1$
2. Assume the claim is true for n . For $n + 1$ pick a unit vector \hat{e}_\perp that is orthogonal to $\hat{\mathbb{1}}$ and construct the unit vector $\hat{e}_{n+1} = \frac{1}{\sqrt{n+1}}\hat{\mathbb{1}} + \sqrt{\frac{n}{n+1}}\hat{e}_\perp$. Clearly \hat{e}_{n+1} satisfies the condition $\langle \hat{e}_{n+1}, \hat{\mathbb{1}} \rangle = \frac{1}{\sqrt{n+1}}$.
3. To use the the induction assumption we construct a new row sum unit vector $\hat{\mathbb{1}}_n = \frac{n}{\sqrt{n^2-n}}\hat{\mathbb{1}} - \sqrt{\frac{n}{n^2-n}}\hat{e}_\perp$ in one dimension lower by projecting onto the subspace orthogonal to \hat{e}_{n+1} .
4. By the induction assumption there exists a basis \hat{e}_i with $i \leq n$, such that $\langle \hat{e}_i, \hat{\mathbb{1}}_n \rangle = \frac{1}{\sqrt{n}}$
5. Because \hat{e}_i with $i \leq n$ was constructed in the space orthogonal to \hat{e}_{n+1} it follows that $\langle \hat{e}_i, \hat{e}_j \rangle = \delta_{ij}$ for all $i, j \leq n + 1$.
6. Then using the definitions of \hat{e}_{n+1} and $\hat{\mathbb{1}}_n$ we can calculate the inner product $\langle \hat{e}_i, \hat{\mathbb{1}}_n \rangle$ for $i \leq n$

$$\begin{aligned}
\frac{1}{\sqrt{n}} &= \langle \hat{e}_i, \hat{\mathbb{1}}_n \rangle \\
&= \frac{n}{\sqrt{n^2-n}} \langle \hat{e}_i, \hat{\mathbb{1}} \rangle - \sqrt{\frac{n}{n^2-n}} \langle \hat{e}_i, \hat{e}_\perp \rangle \\
&= \frac{\sqrt{n^3+n^2} + \sqrt{n}}{\sqrt{n^3-n}} \langle \hat{e}_i, \hat{\mathbb{1}} \rangle - \sqrt{\frac{n}{n^2-n}} \langle \hat{e}_i, \hat{e}_{n+1} \rangle
\end{aligned}$$

Inverting the fraction in the equality yields $\langle \hat{e}_i, \hat{\mathbb{1}} \rangle = \frac{1}{\sqrt{n+1}}$

□

To establish the central result of this chapter, that the algebraic closure of the matrices C_{ij} is the stochastic Lie algebra $\mathfrak{st}(\hat{\mathbb{I}})$, we need a preliminary result that proves the commutators $[C_{ij}, C_{kl}]$ are linear combinations of matrices C_{ij}

Lemma 4.

$$C_{ij}C_{kl} = \begin{cases} -C_{il} & i = k, \\ C_{il} - C_{ij} & j = k, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. We proceed in two steps; calculating the terms of the products, then simplifying the cases, always assuming $i \neq j$ and $k \neq l$.

1. Term wise computation yields

$$\begin{aligned} C_{ij}C_{kl} &= \hat{e}_i \otimes (\hat{e}_j - \hat{e}_i) \hat{e}_k \otimes (\hat{e}_l - \hat{e}_k) \\ &= \hat{e}_i \otimes \hat{e}_j \hat{e}_k \otimes \hat{e}_l + \hat{e}_i \otimes \hat{e}_i \hat{e}_k \otimes \hat{e}_k - \hat{e}_i \otimes \hat{e}_j \hat{e}_k \otimes \hat{e}_k - \hat{e}_i \otimes \hat{e}_i \hat{e}_k \otimes \hat{e}_l \\ &= \delta_{jk} \hat{e}_i \otimes \hat{e}_l + \delta_{ik} \hat{e}_i \otimes \hat{e}_k - \delta_{jk} \hat{e}_i \otimes \hat{e}_k - \delta_{ik} \hat{e}_i \otimes \hat{e}_l \\ &= (\delta_{jk} - \delta_{ik}) \hat{e}_i \otimes (\hat{e}_l - \hat{e}_k) \end{aligned}$$

2. We work through each case of $\delta_{jk} - \delta_{ik}$, starting with the case $i = k$

$$\begin{aligned} C_{ij}C_{il} &= (\delta_{jk} - \delta_{ii}) \hat{e}_i \otimes (\hat{e}_l - \hat{e}_i) \\ &= -\hat{e}_i \otimes (\hat{e}_l - \hat{e}_i) \\ &= -C_{il} \end{aligned}$$

3. When $j = k$ we have

$$\begin{aligned}
C_{ij}C_{jl} &= (\delta_{jj} - \delta_{ij}) \hat{e}_i \otimes (\hat{e}_l - \hat{e}_j) \\
&= \hat{e}_i \otimes (\hat{e}_l - \hat{e}_j) \\
&= \hat{e}_i \otimes (\hat{e}_l - \hat{e}_i + \hat{e}_i - \hat{e}_j) \\
&= C_{il} - C_{ij}
\end{aligned}$$

4. Finally when none of the previous conditions apply

$$\begin{aligned}
C_{ij}C_{kl} &= (\delta_{jk} - \delta_{ik}) \hat{e}_i \otimes (\hat{e}_l - \hat{e}_k) \\
&= 0 \cdot \hat{e}_i \otimes (\hat{e}_l - \hat{e}_k) \\
&= 0
\end{aligned}$$

□

While this result is sufficient to accomplish the central result, it is worth carrying through with a computation of the structure constants of the generators.

Corollary 1.

$$[C_{ij}, C_{kl}] = \begin{cases} C_{ij} - C_{il} & i = k, \\ C_{kj} - C_{ki} & i = l, \\ C_{il} - C_{ij} & j = k, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. As in the previous lemma we work case wise through the equalities.

1. Starting with $i = k$

$$\begin{aligned}
[C_{ij}, C_{il}] &= C_{ij}C_{il} - C_{il}C_{ij} \\
&= C_{ij} - C_{il}
\end{aligned}$$

2. For $i = l$

$$\begin{aligned}[C_{ij}, C_{ki}] &= C_{ij}C_{ki} - C_{ki}C_{ij} \\ &= C_{kj} - C_{ki}\end{aligned}$$

3. For $j = k$

$$\begin{aligned}[C_{ij}, C_{jl}] &= C_{ij}C_{jl} - C_{jl}C_{ij} \\ &= C_{il} - C_{ij}\end{aligned}$$

4. When none of the conditions apply

$$\begin{aligned}[C_{ij}, C_{kl}] &= C_{ij}C_{kl} - C_{kl}C_{ij} \\ &= 0\end{aligned}$$

□

We can now proceed with the central result that motivates this chapter.

Theorem 1. *The canonical generators of $\mathfrak{st}(\hat{\mathbb{I}})$ are $C_{ij} = \hat{e}_i \otimes (\hat{e}_j - \hat{e}_i)$*

Proof. The previous lemma has established that the products, and thus the commutators, of C_{ij} are linear in C_{ij} . We then have to prove that the smallest algebra that contains C_{ij} is $\mathfrak{st}(\hat{\mathbb{I}})$. As thus, it is sufficient to prove that matrices C_{ij} form a basis for $\mathfrak{st}(\hat{\mathbb{I}})$. This is because a necessary condition for an algebra to contain the matrices C_{ij} is that it must contain all sums of the matrices C_{ij} . If one could sum their way out of the algebra then it would not be an algebra.

1. That $\mathfrak{st}(\hat{\mathbb{I}})$ is an $n^2 - n$ dimensional vector space should be clear from the previous discussion. A full formal proof of this claim is found through induction on the dimension n .

2. The matrices C_{ij} are in $\mathfrak{st}(\hat{\mathbb{1}})$. From the definition of the canonical generators

$$\begin{aligned} C_{ij}\hat{\mathbb{1}} &= \hat{e}_i \otimes (\hat{e}_j - \hat{e}_i) \hat{\mathbb{1}} \\ &= \hat{e}_i (\langle \hat{e}_j, \hat{\mathbb{1}} \rangle - \langle \hat{e}_i, \hat{\mathbb{1}} \rangle) \\ &= \hat{e}_i \left(\frac{1}{\sqrt{n}} - \frac{1}{\sqrt{n}} \right) \\ &= 0 \end{aligned}$$

3. C_{ij} is a set of $n^2 - n$ linear independent matrices and so must form a basis for all of $\mathfrak{st}(\hat{\mathbb{1}})$. That there are only $n^2 - n$ matrices is clear from the fact that $C_{ii} = 0$. While the formal proof of linear independence is again found through induction on the dimension n .

□

The previous theorem serves as the definition of a set of canonical generators of $\mathfrak{st}(\hat{\mathbb{1}})$. It is important to note that neither the basis \hat{e}_i nor the canonical generators C_{ij} are unique. They are uniquely defined only up to rotations orthogonal to the vector $\hat{\mathbb{1}}$.

Before moving on it is worth briefly revisiting the distinction between the standard convex polytope of stochastic matrices and the stochastic Lie group, to develop some physical intuition into the relationship between the two sets of matrices which have a non-trivial and geometrical interesting intersection.

Corollary 2. $\exp(\alpha C_{ij}) = I + (1 - e^{-\alpha}) C_{ij}$

Proof. From the definition of the matrix exponential

$$\begin{aligned} \exp(\alpha C_{ij}) &= \sum_{n=0}^{\infty} \frac{1}{n!} \alpha^n C_{ij}^n \\ &= I + \sum_{n=1}^{\infty} \frac{1}{n!} (-1)^{n+1} \alpha^n C_{ij} \\ &= I + (1 - e^{-\alpha}) C_{ij} \end{aligned}$$

□

This last corollary admits a pleasant heuristic interpretation: that each canonical generator C_{ij} can be thought of as measuring the infinitesimal flow of probability from the state represented by basis element \hat{e}_i to the state represented by the basis element \hat{e}_j . This can be seen by considering the matrix representation of $\exp(\alpha C_{ij})$ in the basis spanned by \hat{e}_i and \hat{e}_j .

$$\begin{aligned} I + (1 - e^{-\alpha}) C_{ij} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + (1 - e^{-\alpha}) \begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} e^{-\alpha} & 1 - e^{-\alpha} \\ 0 & 1 \end{pmatrix} \end{aligned}$$

The basis elements \hat{e}_i represent the states of a continuous Markov process on a finite state space; in that when the multipliers of the canonical generators are positive the matrix exponential gives a proper transition matrix the process. The reverse is also true, and can be summarized in the following corollary.

2.2 Doubly Stochastic Matrices

Doubly stochastic matrices require double conservation of the vector $\hat{\mathbb{1}}$, leaving only $(n - 1)^2$ linear degrees of freedom. This is an important clue in the construction of a canonical representation. In fact the representation can be found by choosing one additional vector \hat{e}_n to “omit”. This vector plays a similar role to the diagonal in the previous construction and is used to balance the row and column sums back to zero. $St(\hat{\mathbb{1}}, \hat{\mathbb{1}})$ and $\mathfrak{st}(\hat{\mathbb{1}}, \hat{\mathbb{1}})$

Chapter 3

Padé Approximation of Derivatives of the Exponential Map

3.1 The Gradient

3.1.1 Algebraic Formulation

3.1.2 Algorithm

3.2 The Hessian

3.2.1 Algebraic Formulation

3.2.2 Algorithm

Chapter 4

Maximum Likelihood Estimation from First Hitting Times

4.1 Distribution of First Hitting Times

4.2 The Likelihood and Its Maximization

4.3 Newton-Raphson Maximization

4.3.1 Formulation

4.3.2 Algorithm

Chapter 5

Conclusion

5.1 Summary of Results

Review findings

5.2 Discussion

Application of Lie Theory to the embedding problem for first hitting times... Differentiate between problem of choosing a branch of the matrix logarithm and multiple Markov models having the same first hitting time distribution. Once a principle branch of the logarithm is fixed stochastic Lie algebra can give meaning to the idea of a simplest model, the one expressed in the fewest canonical generators.

Appendix A

Julia Implementations

Code dumps of implementations of the algorithms in Julia.