#### UNIVERSITY OF CALGARY

The Application of Lie Algebras 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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#### **Abstract**

Continuous time Markov processes and Lie algebras 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 algebra theory will fruitfully yield novel computational methods for estimation problems in continuous time Markov processes. In this project we derive the minimal Lie algebra that contains the generators of a continuous time Markov process, and then using the guarantees of algebraic closure construct a Newton-Raphson algorithm for maximum likelihood estimation of the generator of a continuous time Markov process 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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Symbol Definition

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# Background

- 1.1 Continuous Time Markov Process
- 1.1.1 Stopped Processes
- 1.1.2 Phase Type Distributions and Birth Death Processes
- 1.1.3 Baum-Welch and Viterbi Algorithms
- 1.2 Lie Algebras and the Exponential Map
- 1.2.1 Lie Groups
- 1.2.2 Lie Algebras
- 1.2.3 The Exponential Map

## Lie Algebra of the Generators of Continuous Time Markov

#### **Processes**

#### 2.1 Canonical Representation of the Generators of a Markov Process

#### 2.1.1 Stochastic Matrices

The classical Lie Algebras of physics, like the infinitesimal symmetries of the special unitary algebra  $\mathfrak{su}(n)$ , can all be defined in terms of invariants of a Banach space, such as the matrix invariants of the determinant, trace, or norm. In contrast stochastic matrices are always characterized with respect to a chosen vector, which we will denote  $\hat{\mathbb{1}}$ , for reasons that will become clear later. For an  $n \times n$  matrix this serves as n linear constraints, leaving  $n^2 - n$  linear degrees of freedom.

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

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

**Definition 2.** Let  $\mathfrak{st}(\hat{1})$  denote the Lie algebra of  $St(\hat{1})$ 

**Lemma 2.** The canonical generators of  $\mathfrak{st}(\hat{1})$  are  $C_{ij} = \frac{1}{\sqrt{2}}\hat{e}_i \otimes (\hat{e}_j - \hat{e}_i)$ 

The previous lemma serves as the definition of the canonical generators of  $\mathfrak{st}(\hat{\mathbb{1}})$ .

**Lemma 3.**  $\exp(C_{ij}) = e$ 

Lemma 4.  $C_{ij}C_{kl}=\delta$ 

#### 2.1.2 Doubly Stochastic Matrices

Doubly stochastic matrices require double conservation of the vector  $\hat{1}$ , 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.  $St(\hat{1}, \hat{e}_n)$  and  $\mathfrak{st}(\hat{1}, \hat{e}_n)$ 

## 2.2 Structure Constants of the Generator Algebra

- 2.2.1 Stochastic Matrices
- 2.2.2 Doubly Stochastic Matrices

# Padé Approximation of Derivatives of the Exponential Map

- 3.1 The Gradient
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- 3.2 The Hessian
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# **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
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# Appendix A

# **Julia Implementations**

Code dumps of implementations of the algorithms in Julia.