The University of Chicago
Department of Statistics

STATISTICS COLLOQUIUM

SERGIO BACALLADO

Biophysics Group
Stanford University

Bayesian Analysis of Reversible Markov Chains with Applications to Molecular Dynamics

MONDAY, January 30, 2012, at 4:00 PM
133 Eckhart Hall, 5734 S. University Avenue
Refreshments following the seminar in Eckhart 110.

ABSTRACT

Reversible Markov chains are a simple stochastic model for dynamical systems whose equations of motions are invariant to a sign change in time. In the field of molecular dynamics simulation, they have been applied with much success to model conformational transitions in proteins and nucleic acids. Diaconis and Rolles introduced a conjugate prior which greatly facilitates the inference of reversible Markov models from time series in a finite space.

I will discuss two generalizations of this analysis. In the first part of the talk, I will introduce a three-parameter extension of the prior by Diaconis and Rolles, defined via a reinforced random walk with certain exchangeability properties, which guarantee a de Finetti-style representation as a mixture of Markov chains. This random walk also generalizes two well-known exchangeable urn schemes whose de Finetti measures are the Dirichlet process and the Pitman-Yor process. The extra parameters yield desirable flexibility and facilitate sharing statistical strength between transitions from different states. In addition, the process is defined on infinite spaces, which makes it possible to treat the problem of species sampling from a reversible Markov chain nonparametrically. I will discuss why this is relevant in applications through examples.

In the second part of the talk, I will discuss a generalization of the analysis of Diaconis and Rolles to variable-order Markov chains, which preserves much of the computational tractability of the original. This extension allows us to apply and compare reversible models with different lengths of memory without sacrificing all statistical parsimony.

For further information and inquiries about building access for persons with disabilities, please contact Dan Moreau at 773.702.8333 or send him an email at dmoreau@galton.uchicago.edu. If you wish to subscribe to our email list, please visit the following website:
https://lists.uchicago.edu/web/arc/statseminars.