Department of Mathematics,
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Seminar on Mathematics for Complex Biological Systems

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UCSD

Reflected Diffusions and (Bio)Chemical Reaction Networks

Abstract:

Continuous-time Markov chain models are often used to describe the stochastic dynamics of networks of reacting chemical species, especially in the growing field of systems biology. Discrete-event stochastic simulation of these models rapidly becomes computationally intensive. Consequently, more tractable diffusion approximations are commonly used in numerical computation, even for modest-sized networks. However, existing approximations (e.g., linear noise and Langevin), do not respect the constraint that chemical concentrations are never negative.

In this talk, we propose an approximation for such Markov chains, via reflected diffusion processes, that respects the fact that concentrations of chemical species are non-negative. This fixes a difficulty with Langevin approximations that they are frequently only valid until the boundary of the positive orthant is reached. Our approximation has the added advantage that it can be written down immediately from the chemical reactions. This contrasts with the linear noise approximation, which involves a two-stage procedure — first solving a deterministic ordinary differential equation, followed by a stochastic differential equation for fluctuations around those solutions.

Under mild assumptions, we first prove that our proposed approximation is well defined for all time. Then we prove that it can be obtained as the weak limit of a sequence of jump-diffusion processes that behave like the Langevin approximation in the interior of the positive orthant and like a rescaled version of the Markov chain on the boundary of the orthant. For this limit theorem, we adapt an invariance principle for reflected diffusions, due to Kang and Williams, and modify a result on pathwise uniqueness for reflected diffusions, due to Dupuis and Ishii. Some numerical examples illustrate the advantages of our approximation over direct simulation of the Markov chain or use of the linear noise approximation.

Joint work with Saul Leite (Federal University of Juiz de Fora, Brazil), David Anderson (U. Wisconsin-Madison) and Des Higham (U. Strathclyde).

Organizers: Li-Tien Cheng, Bo Li, and Ruth Williams

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