COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

System Identification of Continuous Time Compartment Models using the Neural Chemical Langevin Equation

KRYSTIAN GANKO

Massachusetts Institute of Technology

ABSTRACT:

Certain chemical and biological systems of practical interest are experimentally observed to have both deterministic drift and diffusive noise structure at low particle numbers, e.g., crystal nucleation and enzymatic reaction. State-space stochastic differential equations (SDEs) model this noise in continuous time, to more realistically describe the stochastic dynamics compared to ordinary differential equation (ODE) descriptions that employ the continuum approximation with no process noise description. Moreover, for applications where process data is bountiful, but the physics are poorly understood, neural networks may be embedded in the state-space dynamics to help identify the system structure (i.e., in the manner of neural state space models). However, identifying structured noise from sampled process data in this fashion often leads to practical identifiability issues, wherein the learned noise models will potentially be strongly biased and uninformative.

This work explores the neural Chemical Langevin Equation (NCLE) in the system identification of compartment models with structured colored noise. Compared to the corresponding neural SDE (NSDE) which uses a biased white noise model, the NCLE offers a parameterization for the drift and diffusion structure with fewer parameters. With the help of the Julia programming language, we construct the NCLE and NSDE variants and deploy a particle filter-based inference approach to calibrate the models on synthetic noisy measurement data. We then compare the predictive performance of both models, and we finally remark on the system identification benefits when using the NCLE model structure variant.

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