



THE UNIVERSITY OF
CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS
STUDENT SEMINAR

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Dynamical Galerkin Approximation: Combining Machine Learning,
Dynamical Systems, and Chemistry

THURSDAY, November 15, 2018, at 1:00 PM
Jones 226, 5747 South Ellis Avenue

ABSTRACT

Understanding chemical dynamics requires estimating complicated dynamical statistics such as expected hitting times, reaction rates, and committor probabilities. In systems with well-defined metastable states and free energy barriers, these quantities can often be numerically estimated by a standard technique. One projects the data onto one or two representative coordinates known as collective variables, and then applies classical rate theories. However, complex processes such as protein folding or the dynamics of disordered proteins generally do not have known one or two dimensional descriptions. These problems require new methods for getting dynamical information.

To address this, we note that many dynamical quantities can be written as the solutions to operator equations using a dynamical operator known as the generator. While for most systems the generator operator is unknown, we show that one can still solve these equations using Monte Carlo. Our method only requires short dynamical trajectories to recover estimates of long-time statistics that converge to the true solution. We give numerical examples showing that DGA can give good results even when the collective variable space is high-dimensional, or incomplete.