LEARNING COLLECTIVE VARIABLES FOR COMPLEX SYSTEMS: A THEORETICAL AND PRACTICAL PERSPECTIVE

CHRISTOF SCHÜTTE

This talk develops a theoretical framework for identifying optimal collective variables (CVs) in complex dynamical systems modeled as high-dimensional Markov processes. The authors define the effective dynamics associated with a CV map and show that optimal CVs minimize the Kullback-Leibler divergence between the full and effective dynamics. The framework establishes error estimates for approximating dominant timescales and transition rates, offering criteria for CV optimality. A key result shows that CVs that are optimal for effective dynamics solve a relative entropy minimization problem. The presentation bridges theoretical insights with data-driven approaches, revealing connections to alternative methods for learning CVs. The findings provide a unified basis for interpreting and improving algorithms in molecular kinetics and related fields.