

COMPUTING COMMITTOR FUNCTION AND INVARIANT DISTRIBUTION FOR RANDOMLY
PERTURBED DYNAMICAL SYSTEMS

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The committor function is a central object in understanding transitions between metastable states in complex systems. It has a simple mathematical description – it satisfies the backward Kolmogorov equation. However, computing the committor function for realistic systems at low temperature is a challenging task, due to the curse of dimensionality and the scarcity of transition data. In this talk, I will present a computational approach that overcomes these issues and achieves good performance on complex benchmark problems with rough energy landscapes. The new approach combines deep learning, importance sampling and feature engineering techniques. I will also discuss the computation of invariant distributions from short trajectories using deep learning.

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