THE UNIVERSITY OF HONG KONG

Institute of Mathematical Research
Department of Mathematics

Numerical Analysis Seminar

Optimal Control Formulation of Transition Path Problems for Markov Jump Processes

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Abstract

Among various rare events, such as biochemical reactions, protein folding, genetic evolution, and quantum tunneling, effectively computing transition paths that connect metastable states in stochastic models is a significant challenge. In this talk, we propose a stochastic optimal control formulation for transition path problems in an infinite time horizon for Markov jump processes on a Polish space. This approach employs an unbounded terminal cost at a stopping time and a controlled transition rate for the jump process to facilitate the transition between metastable states. The running cost is expressed as an entropy form of the control velocity, contrasting with the quadratic form typically used for diffusion processes. Utilizing the Girsanov transformation for Markov jump processes, we integrate the optimal control problem in both finite and infinite time horizons with a stopping time into a unified framework. This framework focuses on the optimal change of measures in the Càdlàg path space by minimizing their relative entropy. We demonstrate that the committor function, derived from the backward equation with appropriate boundary conditions, provides an explicit formula for both the optimal path measure and the associated optimal control for the transition path problem. The presence of an unbounded terminal cost leads to a singular transition rate (unbounded control velocity). To address this, we apply the Gamma convergence technique to regularize the optimal path measure. The limiting path measure is proven to solve a Martingale problem with an optimally controlled transition rate, and the associated optimal control is determined through Doob-h transformation. Consequently, the optimally controlled process realized can almost surely facilitate the transitions.

Date:	Nov. 20, 2023 (Monday)
Time:	11:00am – 12:00noon
Venue:	Room 210, Run Run Shaw Building HKU

All are welcome