Translational AI Center (TrAC) Seminar
Fall 2024

Krishna Garikipati

December 11th at 11:00 AM (US Central Time)

Location and zoom link: https://trac-ai.iastate.edu/event/trac-seminar-series-krishna-garikipati/

Fokker-Planck-Inverse Reinforcement Learning: A physics-constrained approach to Markov Decision Process models of cell dynamics

Abstract

Inverse Reinforcement Learning (IRL) is a compelling technique for revealing the rationale underlying the behavior of autonomous agents. IRL seeks to estimate the unknown reward function of a Markov decision process (MDP) from observed agent trajectories. However, IRL needs a transition function, and most algorithms assume it is known or can be estimated in advance from data. It therefore becomes even more challenging when such transition dynamics is not known a-priori, since it enters the estimation of the policy in addition to determining the system's evolution. When the dynamics of these agents in the state-action space is described by stochastic differential equations (SDE) in It\^{o} calculus, these transitions can be inferred from the mean-field theory described by the Fokker-Planck (FP) equation. We conjecture there exists an isomorphism between the time-discrete FP and MDP that extends beyond the minimization of free energy (in FP) and maximization of the reward (in MDP). We identify specific manifestations of this isomorphism and use them to create a novel physics-aware IRL algorithm, FP-IRL, which can simultaneously infer the transition and reward functions using only observed trajectories. We employ variational system identification to infer the potential function in FP, which consequently allows the evaluation of reward, transition, and policy by leveraging the conjecture. We demonstrate the effectiveness of FP-IRL by applying it to a synthetic benchmark and a biological problem of cancer cell dynamics, where the transition function is inaccessible. This is joint work with Changyang Huang, Siddhartha Srivastava, Kenneth Ho, Kathryn Luker, Gary Luker and Xun Huan.

Short Bio

Krishna Garikipati obtained his PhD at Stanford University in 1996, and after a few years of post-doctoral work, he joined the University of Michigan in 2000, rising to Professor in the Departments of Mechanical Engineering and Mathematics. Between 2016 and 2022, he served as the Director of the Michigan Institute for Computational Discovery & Engineering (MICDE). In January 2024 he moved the Department of Aerospace and Mechanical Engineering at University of Southern California. His research is in computational science, with applications drawn from biophysics, materials physics, mechanics and mathematical biology. Of recent interest are data-driven approaches to computational science. He has been awarded the DOE Early Career Award for Scientists and Engineers, the Presidential Early Career Award for Scientists and Engineers (PECASE), and a Humboldt Research Fellowship. He is a fellow of the US Association for Computational Mechanics, and the International Association for Computational Mechanics, a Life Member of Clare Hall at University of Cambridge, and a visiting scholar in Computational Biology at the Flatiron Institute of the Simons Foundation.

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