

AI with Hamiltonian Mechanics: From Predictions to Understanding

Thursday, 27 February 2025 14:00 (30 minutes)

How do AI and Hamiltonian Mechanics drive each other's advancement, enabling stronger predictions and offering deeper insights? In this presentation, we explore how AI can not only predict but also understand Hamiltonian dynamics. First, we introduce a robust long-term prediction framework that combines an improved Hamiltonian Neural Network with Bayesian data assimilation. This method achieves high accuracy even in 3D environments, showing that AI can become a powerful tool for real-world applications.

Building on these predictive successes, we now ask whether AI can truly understand Hamiltonian mechanics. We introduce operator learning, a method that allows AI to handle mappings in infinite-dimensional spaces, then apply it to Hamiltonian systems. We test whether AI can produce phase space trajectories from an arbitrary potential function without using equations or solvers. Our results show that, under certain conditions, AI can indeed predict these trajectories. Finally, we discuss current limitations, propose future research directions, and consider how AI might advance scientific discovery.

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