Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology

Contribution ID: 24

Type: Contributed Talk (30min)

Solving quantum and classical dissipative dynamics with artificial neural networks

Tuesday 20 September 2022 09:45 (30 minutes)

We develop a variational approach to simulating the dynamics of open quantum and classical many-body systems using artificial neural networks. The parameters of a compressed representation of a probability distribution are adapted dynamically according to the Lindblad master equation or Fokker Planck equation, respectively, by employing a time-dependent variational principle. We illustrate our approach by solving the dissipative quantum Heisenberg model in one and two dimensions for up to 40 spins and by applying it to the simulation of confinement dynamics in the presence of dissipation [1]. Also, we use normalizing flows to variationally solve diffusive classical dynamics in high dimensions [2].

[1] M. Reh, M. Schmitt, M. Gärttner, Phys. Rev. Lett. 127, 230501 (2021)

[2] M. Reh, M. Gärttner, arXiv:2206.01927

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Session Classification: Quantum Many-Body States

Track Classification: Quantum Many Body States