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

Contribution ID: 13

Type: Contributed Talk (15 min)

Unraveling Quantum Scrambling with Neural Networks

Tuesday 20 September 2022 15:30 (15 minutes)

Quantum scrambling is the process by which quantum information is spread within the degrees of freedom of many-body quantum systems. As such, understanding what are the features of a quantum system that maximise this information spreading has become a recent topic of interest of crucial importance. Graph theory provides a natural mathematical framework to encode the interactions of a quantum many-body system, and we thus employ it to study the properties of quantum scrambling as we vary the underlying graph of interactions. Predicting when a particular quantum many-body system features either strong quantum scrambling (chaotic system) or not (integrable system) is a delicate issue where sophisticated computationally expensive methods are needed. We use (i) A Convolutional Neural Network, and (ii) A Graph Neural Network to understand better this integrable-to-chaotic transition and find that suprisingly simple graph-theoretic indices control this transition. In particular, we show that clustering coefficients can be used to predict its scrambling properties. While still a work in progress, we believe our results pave the way for a better understanding of how to maximize the spreading of quantum information in a controlled way.

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Session Classification: Quantum Many-Body States

Track Classification: Quantum Many Body States