ICFO

Congratulations to New ICFO PhD Graduate

Dr Patrick Huembeli graduated with a thesis entitled i¿½Machi e Learning for Quantum Physics and Quantum Physics for Machi e Learningi¿½

March 26, 2021

We congratulate Dr Patrick Huembeli who defended his thesis today in ICFO's auditorium with online participations due to social distancing to contain the Coronavirus pandemic. Dr Huembeli received his MSc in Physics at the University of Basel, Switzerland. He joined the Quantum Information Theory research group led by ICREA Prof at ICFO Dr Antonio Acin to carry out his PhD studies on quantum phase transitions, tensor networks and how to combine them with machine learning. Dr Huembeli's thesis entitled i¿½Machine Learning for Quant m Physics and Quantum Physics for Machine Learning" was supervised by ICREA Prof at ICFO r Antonio Aci

ABSTRACT:

Research at the intersection of machine learning (ML) and quantum physics is a recent growing field due to the enormous expectations and the success of both fields. ML is

arguably one of the most promising technologies that has and will continue to disrupt many aspects of our lives. The way we do research is almost certainly no exception and ML, with its unprecedented ability to find hidden patterns in data, will be assisting future scientific discoveries. Quantum physics on the other side, even though it is sometimes not entirely intuitive, is one of the most successful physical theories and we are on the verge of adopting some quantum technologies in our daily life. Quantum many-body physics is a subfield of quantum physics where we study the collective behavior of particles or atoms and the emergence of phenomena that are due to this collective behavior, such as phases of matter. The study of phase transitions of these systems often requires some intuition of how we can quantify the order parameter of a phase. ML algorithms can imitate something similar to intuition by inferring knowledge from example data. They can, there- fore, discover patterns that are invisible to the human eye which makes them excellent candidates to study phase transitions. At the same time, quantum devices are known to be able to perform some computational task exponentially faster than classical computers and they are able to produce data patterns that are hard to simulate on classical computers. Therefore, there is the hope that ML algorithms run on quantum devices show an advantage over their classical analog.

This thesis is devoted to study two different paths along the front lines of ML and quantum physics. On one side we study the use of neural networks (NN) to classify phases of mater in many-body quantum systems. On the other side, we study ML algorithms that run on quantum computers. The connection be- tween ML for quantum physics and quantum physics for ML in this thesis is an emerging subfield in ML, the interpretability of learning algorithms. A crucial ingredient in the study of phase transitions with NNs is a better understanding of the predictions of the NN, to eventually infer a model of the quantum system and interpretability can assist us in this endeavour. The interpretability method that we study analyzes the influence of the training points on a test prediction and it depends on the curvature of the NN loss landscape. This further inspired an in-depth study of the loss of quantum machine learning (QML) applications which we as well will discuss.

In this thesis we give answers to the questions of how we can leverage NNs to classify phases of matter and we use a method that allows to do domain adaptation to transfer the learned "in- tuition" from systems without noise onto systems with noise. To map the phase diagram of quantum many-body systems in a fully unsupervised manner, we study a method known from anomaly detection that allows us to reduce the human input to a mini- mum. We will as well use interpretability methods to study NNs that are trained to distinguish phases of matter to understand if the NNs are learning something similar to an order parameter and if their way of learning can be made more accessible to humans. And finally, inspired by the interpretability of classical NNs, we develop tools to study the loss landscapes of variational quantum circuits to identify possible differences between classical and quantum ML algorithms that might be leveraged for a quantum advantage.

Thesis Committee:

Prof Dr Evert van Nieuwenburg, Niels Bohr Institute Copenhagen

Prof Dr Tobias Grass, ICFO

Prof Dr Vedran Dunjko, Universiteit Leiden