QI 3: Quantum Machine Learning

Time: Monday 11:00–13:00 Location: B305

Invited Talk QI 3.1 Mon 11:00 B305

Characterising quantum device variability with machine learning — •Natalia Ares — University of Oxford

Machine learning is proving to be essential in the tuning and characterization of quantum devices. The search for operation conditions, which often requires navigating large and complex parameter spaces, can now be fully automated, with performances superior to those achieved by human experts. Now these machine learning approaches are not only enabling scalability by automating qubit control, but also by providing us with unprecedented insight into quantum device variability.

We can use machine learning algorithms for automatic tuning across different semiconductor platforms. This demonstrates not only the robustness of these algorithms against the differences in the characteristics of the material system and device architecture, but that they can provide a tool for their comparison and analysis. I will show that by using a physics-aware machine learning algorithm we are able to infer the disorder potential affecting the operation of quantum dot devices, revealing a hidden characteristic of such devices, and thus narrowing the gap between simulation and reality.

QI 3.2 Mon 11:30 B305

The application of quantum neural networks in function approximation — •David Kreplin and Marco Roth — Fraunhofer IPA, Nobelstraße 12, 70569 Stuttgart, Deutschland

Approximating functions by parameterized quantum circuits is a promising application for quantum computing, since the repetitive encoding of the input data can result in an exponentially growing complexity of the function. In the literature, this approach is often described as Quantum Neural Networks (QNNs), since it can be similarly utilized as classical artificial neural networks.

In this talk, we show how an efficient and general function approximation can be realized by a QNN. We discuss the construction, training, and the application of the QNN with the example of solving a differential equation based model of a hydrogen electrolyzer and benchmark the results against classical neural networks.

A particular focus in this talk will be on the unavoidable noise that results from the finite sampling of the quantum state. This so-called shot noise strongly degrades the training process and yields a noisy outcome of the QNN. We discuss how that shot noise can be strongly reduced during the training of the QNN by an additional regularization term. This not only reduces the noise in the final function but also simplifies the training process on shot based simulators or real devices. Finally, we present results from the real quantum computing hardware and we reflect on the obstacles that we currently face in training such QNNs on the real backends.

QI 3.3 Mon 11:45 B305

Parameterized quantum circuits for reinforcement learning of classical rare dynamics — Alissa Wilms[1,2], •Laura Ohff[2,3], Andrea Skolik[4,5], David A. Reiss[1], Sumeet Khatri[1], and Jens Eisert[1,6,7] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Berlin, Germany — [2]Porsche Digital GmbH, Ludwigsburg, Germany — [3]Otto-Friedrich Universität Bamberg, Bamberg, Germany — [4]Leiden University, Leiden, The Netherlands — [5]Volkswagen Data:Lab, Munich, Germany — [6]Fraunhofer Heinrich Hertz Institute, Berlin, Germany — [7]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

In the study of non-equilibrium or industrial systems, rare events are crucial for understanding the systems' behavior. Since they are atypical, one requires specific methods for sampling and generating rare event statistics in an automated and statistically meaningful way. We propose two quantum reinforcement learning (QRL) approaches to study rare dynamics of time-dependent systems and investigate their benefits over classical approaches based on neural networks. We investigate how architectural choices influence the successful learning by QRL agents and demonstrate that a QRL agent is capable of learning the rare dynamics of a random walker with using just a single qubit. Furthermore, we are able to numerically demonstrate an improved environment exploration during learning and a better performance in coping with environment scaling by the quantum agents in comparison to their classical counterparts.

QI 3.4 Mon 12:00 B305

Optimal storage capacity of quantum Hopfield neural networks — •Lukas Bödeker[1,2], Eliana Fiorelli[1,2,3], and Markus Müller[1,2] — [1]Institute for Theoretical Nanoelectronics (PGI-2), Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [3]Instituto de Fisica Interdisciplinar y Sistemas Complejos (IFISC), CSIC UIB Campus, Palma de Mallorca, E-07122, Spain

Quantum neural networks form one pillar of the emergent field of quantum machine learning. Here, quantum generalisations of classical networks realizing associative memories - capable of retrieving patterns, or memories, from corrupted initial states - have been proposed. It is a challenging open problem to analyze quantum associative memories with an extensive number of patterns, and to determine the maximal number of patterns the quantum networks can reliably store, i.e. their storage capacity. In this work, we propose and explore a general method for evaluating the maximal storage capacity of quantum neural network models. As an example, we apply our method to an open-system quantum associative memory formed of interacting spin-1/2 particles realizing coupled artificial neurons. The system undergoes a Markovian time evolution resulting from a dissipative retrieval dynamics that competes with a coherent quantum dynamics. We map out the non-equilibrium phase diagram and study the effect of temperature and Hamiltonian dynamics on the storage capacity. Our method opens an avenue for a systematic characterization of the storage capacity of quantum associative memories.

QI 3.5 Mon 12:15 B305

Quantum kernel methods for regression — •Jan Schnabel — Fraunhofer-Institut für Produktionstechnik und Automatisierung IPA, Center for Cyber Cognitive Intelligence (CCI), Stuttgart, Germany

It was shown in Refs. [1,2] that encoding data into a quantum state and interpreting the respective expectation value when measuring w.r.t. an observable as machine learning model, links quantum computing to the rich framework of classical kernel theory. Hence, these theoretical tools can now be used to understand quantum models. Here, the inherent structure of quantum kernel methods is particularly suited for NISQ applications. As a result, these facts caused constantly growing research activities in this field, where little attention has been hitherto paid to quantum kernel regression problems.

In this talk, I briefly introduce the core theoretical concepts of different approaches for computing quantum kernels before discussing associated challenges. The latter includes the role of classical data pre-processing and selection, data redundancies as well as the design of quantum feature maps. These aspects are discussed based on project-specific use cases from hydrogen production research. Beyond that, I attempt to provide a systematic comparison of different quantum kernel regression approaches and show results from real backend runs. This also incorporates demonstrating effects of proper error mitigation techniques.

[1] M. Schuld and N. Killoran. Phys. Rev. Lett. 122, 040504 (2019)
[2] M. Schuld, arXiv:2101.11020v2 (2021)

QI 3.6 Mon 12:30 B305

Renormalisation through the lens of QCNNs — •Nathan A. McMahon, Petr Zapletal, and Michael J. Hartmann — Friedrich-Alexander-Universität Erlangen- Nürnberg

The cluster-Ising model is an example of a quantum model with a symmetry protected topological (SPT) phase. For this model, the efficiency of performing phase recognition has recently been improved over measuring string order parameter (SOP) by the use of a particular quantum convolutional neural network (QCNN), which was motivated by renormalisation theory.

Unlike most neural networks, the function of the QCNN used here is relatively straightforward to explain. First, each layer of the QCNN performs a process analogous to both renormalisation/quantum error correction. Second, the remainder of the circuit simply determines if we are in the ground state of a stabiliser Hamiltonian. If the energy is sufficiently low we consider the input state to be in the target phase.

This QCNN also has a second feature, it is exactly equivalent to a constant depth quantum circuit + post-processing. Beyond just providing a cheaper circuit, this also points to the generalisation of phase

recognising QCNNs beyond the cluster-Ising model. Combining these with the fidelity view of quantum phases, I will discuss the potential of QCNNs as a quantum information theory construction of renormalisation.

QI 3.7 Mon 12:45 B305

Quantum Gaussian Processes for Bayesian Optimization — •Frederic Rapp and Marco Roth — Fraunhofer IPA, Stuttgart 70569, Nobelstrasse 12

An important aspect of machine learning is finding the best possible hyperparameters for a given model. Bayesian optimization is one often used algorithm when tackling this task. It requires a surrogate model where Gaussian processes can be used. Gaussian processes are a method based on the evaluation of kernel matrices that serve as covariance functions. These matrices can be evaluated using a quantum computer by encoding the data into the quantum Hilbert space. We study Gaussian processes using quantum kernels based on parameterized quantum circuits, and their application to regression tasks, as well as their usage as a surrogate model for Bayesian optimization. We show that the method can solve a regression of a one-dimensional function under the influence of different quantum computing noise sources. We discuss the important aspects of the model and provide an example of the optimization of the method when solving a multi-dimensional regression task. Finally, we perform a hyperparameter tuning using Bayesian optimization based on quantum Gaussian process regression. We show that the quantum version of the algorithm is able to find suitable hyperparameter settings of a given problem that are comparable to applying the classical counterpart and even better than using a random search based algorithm.