FM 90: Special Session: Quantum Physics for AI & AI for Quantum Physics

Time: Friday 11:00–13:00 Location: Audi Max

Invited Talk FM 90.1 Fri 11:00 Audi Max

How to use quantum light to machine learn graph-structured data — •Maria Schuld[1,2], Kamil Bradler[1], Robert Israel[1], Daiqin Su[1], and Brajesh Gupt[1] — [1]Xanadu, Toronto, Canada — [2]University of KwaZulu-Natal, Durban, South Africa

A device called a 'Gaussian Boson Sampler' has initially been proposed as a near-term demonstration of classically intractable quantum computation. But these devices can also be used to decide whether two graphs are similar to each other, which is the central challenge when doing machine learning on data represented by graphs, such as molecules and social networks. In this talk, I will show how to construct a graph similarity measure - or 'graph kernel' as it is known in machine learning - using samples from an optical Gaussian Boson Sampler. Combining this with standard machine learning methods allows us to predict features of the graph using example data. I will present promising benchmark results comparing the 'quantum kernel' to 'classical kernels' and motivate theoretically why such a continuous-variable quantum computer can actually extract interesting properties. The work is an example of how to use first-generation quantum technologies for machine learning tasks.

Invited Talk FM 90.2 Fri 11:30 Audi Max

Ensuring safety for AI methods - from basic research to Bosch applications — •David Reeb — Bosch Center for Artificial Intelligence, Renningen, Germany

For industry and business applications - especially for safety critical ones - which involve machine learning, it is imperative to ensure that such data-driven methods perform as promised, despite the fact that only a small part of reality has been seen during training. I will motivate this need via Bosch applications, and then describe theoretical methods to ensure such safety requirements. In particular, I will introduce the framework of Statistical Learning Theory, which provides probabilistic guarantees of this kind, and outline some of its paradigmatic results as well as major open questions. Finally, I will describe how generalization bounds from this theory can be used to devise learning algorithms that yield good safety guarantees. We have employed such a result to train Gaussian Processes - a machine learning method popular in industry - and obtained significantly better generalization guarantees compared to training with conventional methods (arXiv:1810.12263).

Invited Talk FM 90.3 Fri 12:00 Audi Max

Boltzmann machines and tensor networks for simulating quantum many body systems — •Frank Verstrate — Ghent University

I will discuss challenges and opportunities for simulating strongly correlated quantum many body systems using Boltzmann machines and tensor networks.

Invited Talk FM 90.4 Fri 12:30 Audi Max

Response operators in Machine Learning: Response Properties in Chemical Space — •Anders Christensen — Institute of Physical Chemistry and National Center for Computational Design and Discovery of Novel Materials (MARVEL), Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland

This talk focuses on the use of response operators in machine learning models for properties of chemical compounds. The role of response operators is well-established in quantum chemistry in which they are used to calculate properties of chemical compounds using differential operators. The same response operators commonly used in quantum chemistry are here applied to a new machine learning model in order to increase its accuracy. Prediction errors for corresponding properties reach high accuracies for small training set sizes. For example, the learning rate of dipole moments is improved by a factor 20x compared to a similar model without operators. In addition, the prediction of vibrational normal modes and infrared spectra of small molecules demonstrates the applicability of this approach for chemistry. The presented operator-based approach is general and can in principle be applied to any machine learning model.