# Machine Learning in Quantum Science

*This manifesto is a call for European funding of research at the interface of machine learning (ML) and quantum science as a foundation of future key technologies.*

***Why machine learning in quantum science?***

The origins of the on-going machine learning revolution can be traced back to the rapid development of unprecedented computational power in combination with the availability of large data following the advent of the internet. Machine learning has already started shaping our everyday lives, as evidenced not least by powerful language models such as chatGPT. At the same time, it is being used ubiquitously bringing new advances across various disciplines, including the natural sciences, where it is, e.g., revolutionising the prediction of protein folding.

A prime match for the machine-learning revolution is quantum science, which is a thriving research field with near-term applications of huge impact, including quantum technologies as well as new functional materials for renewable energy systems or molecules that can serve as drugs or fertilisers. It is becoming apparent that machine learning techniques can greatly boost these activities and push them to another level of efficiency. Besides developments with foreseeable applications, machine learning techniques have the potential to also shape our approach to fundamental physics.

Quantum physics is a data- and computation-intensive science that naturally matches the proven strengths of modern machine learning tools. Conversely, quantum devices can be used to process and analyse data in radically new ways and thus have the unique potential to bring the inner workings of machine learning to a fundamentally different level. For these reasons, research at the close interface of quantum science and machine learning should be given particular consideration and attention.

***What advances are to be expected?***

Quantum science has the potential for a large impact by providing the tools to discover new molecules or exotic materials. However, the exponential complexity of quantum systems makes this research program a formidable challenge. Therefore, quantum computing and quantum simulation on dedicated quantum hardware are a promising route to tackle these challenges. While this route is rapidly developing, it is currently still limited to noisy intermediate-scale quantum devices.

Machine learning will make a difference by boosting the full stack of quantum computing ranging from hardware to software. On the hardware side, machine learning techniques can be employed to automate and accelerate the parallel calibration and optimisation of the qubits. On the software side, it provides new means to discover or optimise quantum algorithms and develop compressed error-correction codes via reinforcement learning or through other variational methods. First examples have demonstrated the power of such approaches and call for further research.

### Discovery and optimisation of quantum experiments

While several algorithms with potential quantum advantage exist, their number is still surprisingly small considering the amount of attention to the field - likely, because quantum physics is intrinsically unintuitive for humans. Therefore, variational quantum algorithms or other forms of quantum machine learning have been identified as a promising route to discover new algorithms. Moreover, the routine operation of quantum computers will require new approaches for device design, readout, efficient compilation, detection of noise mechanisms, and error correction. One example of enhanced compilation are ML models that can autonomously learn generic strategies to compress quantum circuits (see figure). This illustrates that the machine learning toolbox provides manifold ingredients that can boost the hybrid quantum-classical operation for these purposes.

In addition, ML is one of the most prominent tools for an efficient interface between classical and quantum systems both for experiment discovery and control as well as for the translation of classical data into a quantum state and the transpilation of classical into quantum algorithms. ML algorithms operating in hybrid classical-quantum hardware will also allow us to harness properties of quantum systems to devise energy-efficient control tasks.

Concrete examples of ML applications:

- Cross-architecture optimisation of quantum devices and quantum experiments
- Hybrid quantum-classical devices and control protocols

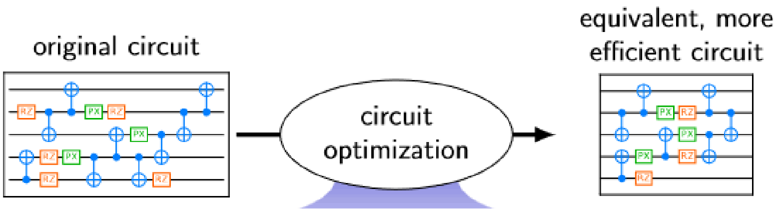



Figure: T. Fösel, M. Y. Niu, F. Marquardt & L. Li. arXiv:2103.07585 (2023)

A second route to applications is currently emerging in the form of advanced ab-initio computational methods enhanced by machine learning: the efficient simulation of certain important classes of complex materials and molecules has come within reach of classical simulations. Ab-initio methods, such as neural-network quantum states, are pushing the state of the art of computational methods, already offering superior precision for some particularly elusive quantum states of matter. This research direction not only demonstrates the key importance of machine learning algorithms for computational quantum science; it also opens new perspectives on the fundamental question of what kind of quantum states can be efficiently represented classically, which is of great importance to quantum information science.

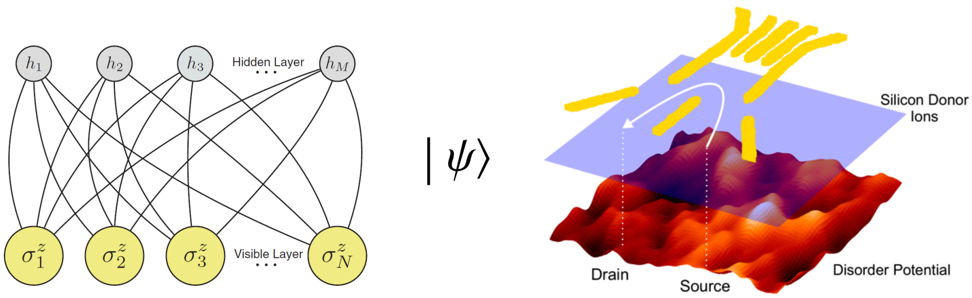
**Simulation of quantum systems**

The simulation of quantum many-particle systems on classical computers is one of the greatest challenges in physics, but extremely important for advances in developing functional materials. It has been demonstrated for a wide range of traditional ab initio methods how machine learning components can be incorporated for their advancement. One example is the encoding of the quantum wave function in the form of artificial neural networks (see figure on the left), which was found to efficiently capture complex quantum states. These methods are currently pushing the state of the art and may be applied to outstanding problems such as high-temperature superconductivity and chemical reaction dynamics.

By combining domain-specific knowledge of quantum mechanics with ML techniques, physics-aware ML can improve the accuracy and interpretability of predictions and models for quantum systems. One example of this is the learning of the hidden disorder landscape of a quantum device (see figure on the right). Developing explainable AI for quantum physics could foster the adoption of quantum machine learning techniques as the paradigm for digital twinning of quantum systems, as well as identify new instances of quantum systems, which are out of reach to simulate with classical ML resources.

Concrete examples of ML applications:

- Neural quantum states
- Automated tailoring of properties of quantum materials
- Digital twins for quantum systems




Figures: G. Carleo & M. Troyer. Science 355, 6325, 602-606 (2017). D. Craig, H. Moon, F. Fedele, D. T. Lennon, B. van Straaten, F. Vigneau, L. C. Camenzind, D. M. Zumbühl, G. A. D. Briggs, M. A. Osborne, D. Sejdinovic & N. Ares. Phys. Rev. X 14, 011001 (2024)

In view of applications as well as fundamental research, data from quantum systems is particularly complex and hard to analyse, since any individual measurement can only provide partial information about the quantum wave function. In traditional approaches information extraction has been guided by experience and physical intuition. Recent work has shown that machine learning tools are very fruitful to further develop our understanding of such data, for example by opening new perspectives through data mining. Leveraging machine learning techniques for pattern recognition and anomaly detection facilitated the identification of quantum phase transitions and similar approaches might allow us to discover unexpected types of order parameters for the characterisation of quantum matter.

With their proven capabilities in strategy discovery, machine learning tools are also extremely powerful for control and feedback cycles of experimental setups and quantum hardware. First examples range from optimised quantum gates on a quantum chip to the faster preparation of atomic Bose-Einstein condensates as a starting point for quantum simulation experiments. Machine learning algorithms open new possibilities to incorporate real-time feedback, the consequences of which we are just starting to understand.

**Analysis of quantum data**

Data from quantum systems is particularly complex and hard to analyse. For instance, in quantum many-body systems, such as correlated electrons in solid-state systems, the relevant order at the basis of their functionality is often hard to extract. Recently it was found that machine learning tools can guide and extend such analysis by an unbiased exploration of all information. For example, artificial neural networks can be used to identify the relevant correlations from snapshots of quantum many-body systems on a lattice (see figure). This can result in the unbiased identification of the essential observables, which is particularly important in noisy settings or for exotic order, where traditional methods fail. In turn, generative modelling can provide crucial support in enriching data from quantum systems where extracting measurements is hardly accessible experimentally, or is particularly time consuming. For that purpose, interpretable and explainable machine learning models will be of particular use to facilitate the discovery and understanding of such new observables.

Concrete examples of ML applications:

- Discovering correlations and symmetries in quantum experiments
- Physics insights through explainable AI and AI-assisted discovery

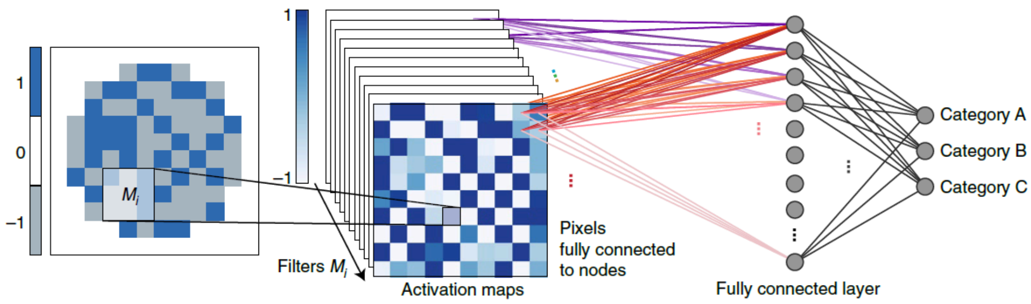



Figure: A. Bohrdt, C. S. Chiu, G. Ji, M. Xu, D. Greif, M. Greiner, E. Demler, F. Grusdt & M. Knap. Nature Physics 15, 921–924 (2019)

Conversely, quantum physics can also feed back to the machine-learning community by providing a vast experience in computational methods. Tailoring new algorithmic tools to the unique challenges of quantum research will enable the creation of synergies that can lead to significant advancements in both fields. For example, the scientific applications will lead to advancements for interpretability and uncertainty quantification of machine learning algorithms that are rooted in the physical domain. Finally, the combination of the fields can lead to a quantum machine learning paradigm that leverages quantum hardware for novel machine learning algorithms themselves. For this to be fruitful, the development of tailored hardware for quantum machine learning protocols will be important.

**Automated calibration of quantum experiments and devices**

Both quantum technologies and fundamental experiments rely on the precise manipulation and fabrication of a large number of quantum degrees of freedom. Common challenges are the efficient characterisation, tuning away of inevitable hardware imperfections, and optimisation of control strategies. As the qubit numbers grow and the applications become manifold, automation becomes essential and machine learning tools have been shown to be powerful for this purpose.

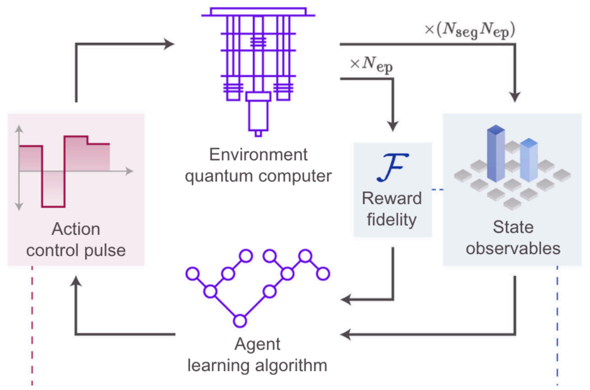



Figure: Y. Baum, M. Amico, S. Howell, M. Hush, M. Liuzzi, P. Mundada, T. Merkh, A. R.R. Carvalho & M. J. Biercuk. PRX Quantum 2, 040324, (2021)

For example, the fully automated tuning of quantum-dot devices faster than human experts was demonstrated. It was also demonstrated in a recent work that the automated optimisation of entangling operations on a superconducting quantum processor could substantially improve their quality (see figure), which is crucial for near-term applications. ML will accelerate the process of quantum state preparation, gate operations, and measurement, leading to faster and more efficient quantum computation or quantum communication protocols. Thus, the ML toolbox can be employed to extend the applicability of quantum devices to problems with many noisy parameters such as imaging, radar, or gravitational wave detection. ML methods can readily be utilised to characterise noise sources.

By facilitating the exploration of large parameter spaces, ML can also be used to design optimised experimental setups for specific quantum tasks, such as quantum communication or quantum computing.

Concrete examples of ML applications:

- Efficient characterisation, tuning, design, and control of quantum experiments
- Mitigation and harnessing noise in quantum systems
- Cross-architecture optimisation of quantum devices; cross-platform certification

Key considerations in applying machine learning to quantum science and technology are *trust*, *robustness*, *interpretability*, and *explainability*. While neural networks (NNs) have shown their power in various applications, their lack of transparency hinders the safe and reliable application of these algorithms to valuable quantum systems. Striking a delicate balance between leveraging advanced algorithms and mitigating risks is crucial for instilling confidence in automated control systems.

**Safety and reliability of controllers**

Safe and reliable application of NN controllers is highly relevant to all fields impacted by automation. To maintain control and ensure device safety, methods must be developed to trust, verify, and potentially limit their capabilities.

<u>Verification:</u> In safety-critical environments, using ML models without verification is infeasible. To reduce the risk of unsafe ML control behaviour, the challenge lies in verifying both the NN controller and the quantum architectures as a cohesive system.
<u>Robustness:</u> Given the inherent noise and slight variations in experimental environments, ensuring the robustness of ML algorithms is paramount. The challenge is to provide robustness analysis for NN controllers, guaranteeing that even small changes in inputs lead to proportional changes in outputs.
<u>Interpretability:</u> An interpretable ML model should empower experts to tune the algorithm post-training based on their knowledge. Neglecting the expertise gained from conducting experiments would be unfortunate. Addressing the challenge involves building interpretable ML models that allow parameter adaptation by experts.
<u>Explainability:</u> Gaining insights into the decision-making process of NN controllers is valuable when employing them. An intriguing challenge to ensure ML model trustworthiness is obtaining explanations of control outputs in understandable human terms.

Additionally, interpretability and explainability of ML in quantum science are critical for uncovering decision mechanisms used by NNs when addressing complex quantum problems. To drive scientific discovery, it is vital to not only comprehend the outputs generated by ML algorithms, but to also understand the underlying principles and concepts that guide their reasoning. Understanding the factors contributing to a model's predictions allows scientists to assess reliability, validate solutions, and identify biases and errors in training data. Ultimately, this improves the robustness of quantum simulations and predictions. Further, extracting human-understandable knowledge from ML models is pivotal for driving breakthroughs in quantum science and technology. Efficient implementation of approaches that effectively contribute to validating findings, uncovering novel insights, and advancing quantum science through new discoveries is a significant challenge.

***What needs to be done to unleash these synergies?***

We believe it is now the right time to invest in research at this emerging interface of quantum science and machine learning so that the European Union (EU) can remain competitive with the US, Canada, and China in developing next-generation quantum technology. Patents for machine learning applications in quantum computing are already picking up speed, but mostly in the US.[1] The quantum flagship has put Europe in a strong position and a broad funding initiative for machine learning in quantum science will enable Europe to take on the lead in these new developing technologies.

Funding needs to be both for fundamental and applied research projects in order to cover the full spectrum of developments. While the applications for optimal control are already being prepared for commercial exploitation by the first start-ups, ab initio computational methods are in a more exploratory phase, which requires funding of purely fundamental research for unleashing the full potential. The same holds for other applications such as the analysis of quantum data arising from experiments that might turn out seminal for our understanding of physics or for future technologies.

Facilitating the exchange between the ML and the quantum physics communities has the potential to transform both fields and interdisciplinary teams are needed to push beyond current boundaries. At the core of our initiative is the merging of diverse communities, to bring together a heterogeneous range of views and ensure openness and diversity. For quantum science and technology to synergise with the field of ML and artificial intelligence, we shall need to bring together quantum experimentalists, quantum theorists, ML engineers, computer scientists, but also entrepreneurs and investors.

Open-source software, freely available and standardised benchmark data sets, model databases, and community challenges were central for the rapid advancement of machine learning techniques. Building on this experience, we believe that creating a similar ecosystem for machine learning in quantum science will likewise boost progress by removing barriers for interdisciplinary collaboration and optimally tapping the available potential. To this end, it is necessary to standardise quantum physics problems through interoperable and structured interfaces. Their role will be to enable sharing of experimental data and translating quantum physics problems into a common ML language. On the one hand, standardisation will enhance the applicability of ML methods in both theoretical and experimental quantum physics, thus improving reusability, reproducibility, and comparability. On the other hand, the development of community-driven projects will create shared spaces, which provide interfaces as tutorials or documentations that

[1] See the Quantum Computing Insight Report of the European Patent Office, page 36.

help students and researchers to familiarise and strengthen cohesion between fields, and encourage interdisciplinary collaboration and cross fertilisation.

Progress in this rapidly developing field requires the training of a next generation of researchers with expertise in quantum science and machine learning, e.g., via suitable doctoral networks. Additional training and educational resources, such as dedicated online platforms and training resources, and encouraging cross-field conferences and symposia, will simplify the access to state-of-the-art ML and further encourage its widespread adoption by quantum scientists. This can bridge the gap between theory and experiment, by facilitating a more seamless integration of theoretical modelling and experimental data analysis. Such educational programmes at the interface of quantum science and machine learning will produce a workforce that is highly skilled in both forward-looking fields. This is not only fruitful for fundamental research, but also essential to keep replenishing industry with open-minded experts who transfer knowledge into competitive products and services.

Social media and science-communication strategies, as well as collaborations with creators, developers, and industry partners, will play a key role in making machine learning techniques in quantum physics beneficial to all of society. By placing engagement at the centre of the research process we shall bridge boundaries between disciplines, facilitate the exchange of valuable knowledge with industry partners and policy makers, and improve the public perception of quantum science.

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