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Book released: Machine Learning in Quantum Sciences

Cambridge University Press has released a new book which introduces the fundamental concepts of Machine Learning applied to Quantum Sciences and offers an overview of this rapidly developing field. The book is addressed to researchers, graduate students and lecturers.

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Artificial intelligence is dramatically reshaping scientific research and is coming to play an essential role in scientific and technological development by enhancing and accelerating discovery across multiple fields. Now, a collaborative effort from world-leading experts has presented a new book, whose main goal is to provide a starting reference for researchers in (quantum) physics and chemistry who want to learn how to apply Machine Learning (ML) and Deep Learning (DL) in their work. It introduces fundamental concepts and offers an overview of this rapidly developing field, where ML is increasingly used for scientific discovery. Among all 29 authors, 9 people are or were ICFO-affiliated, namely**: Dr. Anna Dawid**, **Dr. Borja Requena**, **Dr. Marcin P?odzien**, **Dr. Paolo Stornati**, **Dr. Gorka Munoz-Gil**, **Dr. Patrick Huembeli**, **Prof. Dr. Michal Tomza**, **ICREA Prof. Maciej Lewenstein**, and **Dr. Alexandre Dauphin**.
The book is full of in-depth explanations and detailed presentation of outstanding results that have been obtained through the application of ML in quantum sciences in recent years, such as using Reinforcement Learning for optimal control of quantum experiments and as a tool to optimize quantum circuits, and using neural networks to obtain powerful ansatzes for many-body wave-function, among many others. But it also points at the main limitations and challenges of the field and suggests what next steps should be taken, like developing new methods to explain deep neural networks, and acquire a deeper understanding of the limitations and potential of quantum machine learning.

From transcribed notes to a full book

The original purpose, though, was not to write a full book. This occurred organically later. It all began between August and September of 2021, when Maciej Lewenstein and Alexander Dauphin from ICFO, and Micha? Tomza and Anna Dawid from the Faculty of Physics at the University of Warsaw organized a two-week Summer School on Machine Learning for quantum physics and chemistry, where several talks were given by top experts in the field.

Soon after the workshop, Anna Dawid, at the time a final-year PhD student under Micha? Tomza and Maciej Lewenstein, had the idea to transcribe the lectures and compile them into a set of notes. However, it quickly became clear that raw transcripts weren't sufficient - each topic needed to be expanded. The notes started growing into more and more pages, until Anna and the rest of authors realized that they had enough material for a full book.
The group of volunteers, including workshop organizers, lecturers and participant , coordinated by Anna, then agreed to carry on this long-term project. i¿½Writing this ook was a very bottom-up effort, initiated by a group of enthusiastic researchers who decide to take on the project together. It was a highly collaborative experience, where we all lea ned from each other - not only about the specific scientific topics, but also about ho to coordinate work in a large, distributed teami¿½, shares Dr. Marcin P?odzien, ICFO rese rcher and co-author of the book. And he adds: i¿½The entire project was volunteer-driven, written during our free time, weekends, and holidays, without any official project manager. t was a truly democratic and grassroots initia ive.i¿½ Finally, the first version on arXiv.org appeared in April 2022, and the book appeared published i Cambridge University Press this May 2025

Reference:

Dawid, A., et. al. (2025). Machine Learning in Quantum Sciences. Cambridge University Press.