Machine Learning in Quantum Sciences

Artificial intelligence is reshaping the world, including scientific research. It plays an essential role in scientific discovery by enhancing and accelerating research across multiple fields. This book dives into the interplay between artificial intelligence and the quantum sciences, the outcome of a collaborative effort from the world's leading experts. After presenting the key concepts and foundations of machine learning, a subfield of artificial intelligence, its applications in quantum chemistry and physics are presented in an accessible way, enabling readers to engage with emerging literature on machine learning in science. By examining its state-of-the-art applications, readers will discover how machine learning is currently being applied in their own field and appreciate its broader impact on science and technology.

This book is accessible to undergraduates and more advanced readers from physics, chemistry, engineering, and computer science. Online resources include coding exercises as Jupyter notebooks for self-study of some key topics introduced in the book.

Machine Learning in Quantum Sciences

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In memory of Peter Wittek

Contents

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Evert van Nieuwenburg might be known from the "confusion scheme" or perhaps from TiqTaqToe. He researches ML for quantum systems and often tries to gamify quantum challenges so that AI can learn to play and solve them.

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Sebastian J. Wetzel's research interest is AI in the physical sciences where his most important contributions are related to using ML to calculate phase diagrams and artificial scientific discovery through the interpretation of neural networks.

Preface

We live in fascinating times where scientists are starting to incorporate artificial intelligence (AI) algorithms for knowledge discovery. Advances in this booming field have led to a rapid increase in the interest and confidence of the scientific community in these methods. This trend can be observed by tracking the percentage of machine learning (ML)-based publications in physics, chemistry, and material science, shown in Fig. 0.1. As the number of ML applications grows, keeping track of all advances becomes challenging. Moreover, it is difficult to find reliable intermediate-level learning material that allows one to efficiently bridge the gap between the rapidly developing field of ML and scientists interested in incorporating ML tools into their own research.

The idea of creating this book was born out of *Summer School: Machine Learning in Quantum Physics and Chemistry* that took place between August 23 and September 03, 2021, in Warsaw, Poland. As such, its aim is to give an educational and self-contained overview of modern applications of ML in quantum sciences. The scientific content of this work is inspired by the topics covered by the lecturers and invited speakers of the school. We invite the reader to take a look at the school tutorials in [2] and to reuse the figures prepared for this book, which are available in [3].

The target audience of this book is quantum scientists who want to familiarize themselves with ML methods. Therefore, we assume a basic knowledge of linear algebra, probability theory, and quantum information theory. We also expect familiarity with concepts such as Lagrange multipliers, Hilbert space, and Monte Carlo methods. We also assume that the reader is familiar with quantum mechanics and has a basic grasp of the current challenges in quantum sciences.

Our book is roughly divided into three parts. The first part is devoted to establishing a solid foundation of basic ML concepts needed for understanding its applications in natural sciences. In the second part, we dive into four core application areas of ML in quantum sciences. This covers the use of deep learning and kernel methods in supervised, unsupervised, and reinforcement learning algorithms for phase

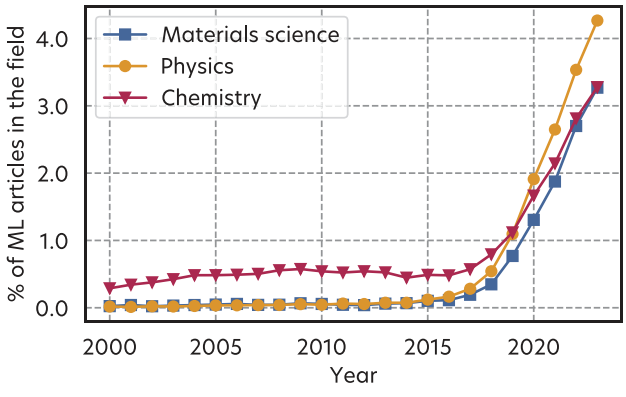

Figure 0.1 The number of ML-based publications in physics, materials science, and chemistry is growing exponentially. Adapted from [1] under the MIT License.

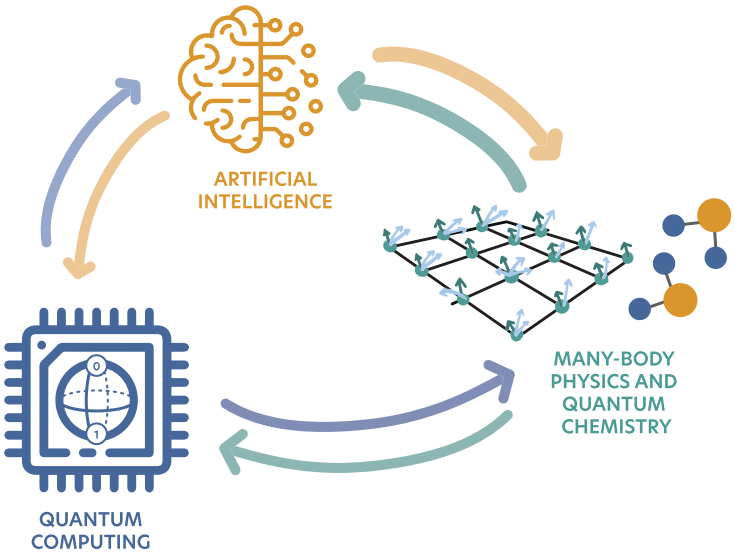

Figure 0.2 Interplay of AI and quantum sciences, in particular quantum computing, many-body physics, and quantum chemistry. Within this book, we focus not only on the influence of AI on quantum sciences but also cover the reverse impact of statistical physics and quantum computing on ML.

classification, representation of many-body quantum states, quantum feedback control, and quantum circuit optimization among other applications. In the third part, we introduce and discuss more specialized topics such as differentiable programming, generative models, statistical physics approaches to ML, and quantum machine learning. All in all, this book discusses the fruitful interplay of AI and quantum sciences, presented schematically in Fig. 0.2.

We do not aim to provide an exhaustive list of ML applications in quantum sciences. Such reviews already exist and nicely summarize the latest achievements [4–6]. Instead, our objective is to provide the reader with enough knowledge, intuition, and tricks of the trade to start implementing ML methods of choice in their own research. As such, we selected the ML applications presented in this work that, we believe, are pedagogically appealing while keeping a broad overview of the field. To this end, we focus on what a reader could do and not only on what has been done. To fulfill this ambition, we conclude each chapter with an outlook and open problems that we recognize as important and promising.

Online resources accompanying this book include coding exercises as Jupyter notebooks for self-study, and focus on key topics introduced in the book. These are available for download at www.cambridge.org/dawidQML.

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Author contributions This manuscript is a result of a unique collaboration between the participants and lecturers of *Summer School: Machine Learning in Quantum Physics and Chemistry* which took place in Warsaw, Poland, during August–September 2021 and which was organized by M. Tomza, A. Dauphin, A. Dawid, and M. Lewenstein. All authors of this manuscript participated in the reading and improvement of its content. In particular:

- *"Introduction"* was written by A. Dawid with the help of M. Płodzień, M. Lewenstein, A. Gresch, R. Koch, B. Requena, and G. Muñoz-Gil.
- *"Basics of machine learning"* was written by A. Dawid, A. Gresch, and J. Arnold with the help of K. Nicoli, K. Donatella, and M. Płodzień.
- *"Phase classification"* was written by J. Arnold, A. Dawid, A. Gresch, R. Koch, M. Płodzień, and S. Wetzel based on the scientific content provided by E. Greplová, P. Huembeli, and S. Wetzel.
- *"Gaussian processes and other kernel methods"* was written by A. Gresch, A. Dawid, K. Nicoli, J. Arnold, R. Krems, and R. A. Vargas-Hernández based on the scientific content provided by R. Krems.
- *"Neural-network quantum states"* was written by K. Donatella, B. Requena, and P. Stornati with the help of R. Okuła and M. Płodzień based on the scientific content provided by G. Carleo, J. Carrasquilla, and F. Vicentini.
- *"Reinforcement learning"* was written by B. Requena, M. Płodzień, and A. Gresch with the help of R. Okuła and G. Muñoz-Gil based on the scientific content provided by V. Dunjko, F. Marquardt, and E. van Nieuwenburg.
- *"Differentiable programming"* was written by J. Arnold, *"Generative models in many-body physics"* – by K. A. Nicoli and M. Gabrié with the help of M. Płodzień, K. Donatella, and A. Dawid, *"Machine learning for experiments"* – by M. Büttner, R. Koch, and A. Dawid, based on the scientific content provided by J. Carrasquilla, E. Greplová, and L. Wang.
- *"Statistical physics for machine learning"* was written by A. Dawid with the help of M. Płodzień based on the scientific content of M. Gabrié, and *"Quantum machine learning"* was written by P. Stornati, A. Dauphin, M. Płodzień, and R. Koch with the help of R. Okuła, based on the lectures of A. Cervera-Lierta and V. Dunjko.
- Finally, *"Conclusions"* was written by A. Dauphin, B. Requena, M. Płodzień, and A. Dawid with the help of all the coauthors.

The project was led by A. Dawid and supervised by A. Dauphin with the help of M. Lewenstein and M. Tomza.

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Note on the text

Numbers and arrays

$\boldsymbol{A}$	matrix
A	tensor
$\boldsymbol{a}$	vector
A	random variable
a	scalar

Physical constants and quantities

β	$1/k_{\mathrm{B}}T$
δ	Kronecker delta
$\langle x \rangle_p$ or $\mathbb{E}[x \mid p]$	estimator of quantity x with respect to distribution p
$\hat{\sigma}$	Pauli matrix
$\hat{H}$	quantum Hamiltonian
$\mathcal{H}$	Hilbert space
σ	spin variable
H	classical Hamiltonian
k_{B}	Boltzmann constant
m	magnetization
Z	partition function

Machine learning quantities

$\boldsymbol{b}$	model biases
K_i or K	ith class or number of classes in a classification problem
$\mathcal{D}$	dataset
n	size of $\mathcal{D}$, that is, the number of training examples
η	learning rate
ϕ	feature map
m	dimensionality of data point $\boldsymbol{x}$, that is, the number of data features
$\hat{f}$	model with converged θ
$\mathcal{L}$	loss (or cost/error) function
$\boldsymbol{H}$	Hessian matrix
d	size of θ, that is, number of model parameters
θ	model parameters
θ^*	converged θ
π	policy
π^*	optimal policy
ℓ_n	L(n) regularization
ς	activation function
$\boldsymbol{w}$ or $\boldsymbol{W}$	vector or matrix of model weights
a	action
D_{KL}	Kullback–Leibler divergence
G	return
r	reward
s	state

Abbreviations

AD automatic differentiation

AE autoencoder

AI artificial intelligence

ANN artificial neural network

AR autoregressive

ARNN autoregressive neural network

BIC Bayesian information criterion

BO Bayesian optimization

CPU central processing unit

CE cross-entropy

CNN convolutional neural network

∂P differentiable programming

DL deep learning

DNN deep neural network

DQN deep Q-network

ECM episodic and compositional memory

GAMP generalized approximate message passing

GAN generative adversarial network

GNS generative neural sampler

GP Gaussian process

GPR Gaussian process regression

GPU graphics processing unit

IGT Ising gauge theory

KRR kernel ridge regression

KL Kullback–Leibler

L-BFGS limited-memory Broyden–Fletcher–Goldfarb–Shanno algorithm

LASSO least absolute shrinkage and selection operator

LE local ensemble

MAE mean absolute error

MAP maximum a posteriori

MCMC Markov chain Monte Carlo

MDP Markov decision process

ML machine learning

MLE maximum likelihood estimation

MPS matrix product state

MSE mean-squared error

NF normalizing flow

NIS neural importance sampling

NISQ noisy intermediate-scale quantum

NMCMC neural Markov chain Monte Carlo

NN neural network

NQS neural quantum state

ODE ordinary differential equation

PC principal component

PCA principal component analysis

PES potential energy surface

POVM positive operator-valued measure

PPT positive under partial transposition

PQC parametrized quantum circuit

PS projective simulation

QAOA quantum approximate optimization algorithm

QD quantum dot

QML quantum machine learning

RBM restricted Boltzmann machine

RKHS reproducing kernel Hilbert space

RL reinforcement learning

RNN recurrent neural network

RUE resampling uncertainty estimation

SGD stochastic gradient descent

SE state evolution

SVM support vector machine

t-SNE t-distributed stochastic neighbor embedding

t-VMC time-dependent variational Monte Carlo

TD temporal difference

TN tensor network

TNS tensor network state

VAE variational autoencoder

VQE variational quantum eigensolver