

# Quantum Machine Learning

## Data Science in Fundamental Physics and its bridge to industry & society

Elías F. Combarro

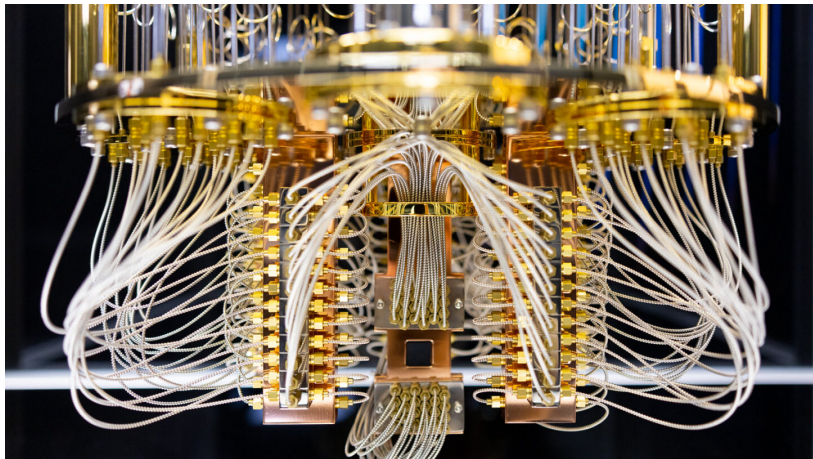
Computer Science Department - University of Oviedo (Spain)

June the 6th 2024

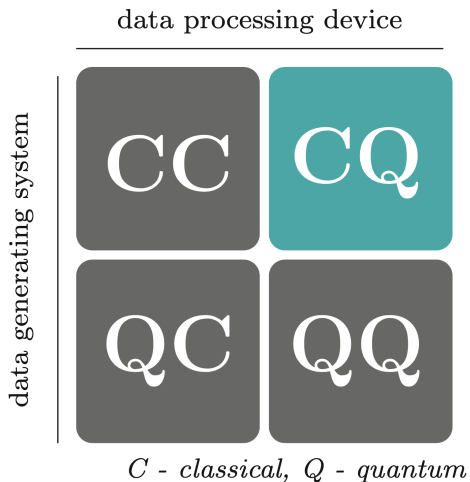


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# The quantum computing revolution?



# What is quantum machine learning?



# Quantum speedups for classical machine learning

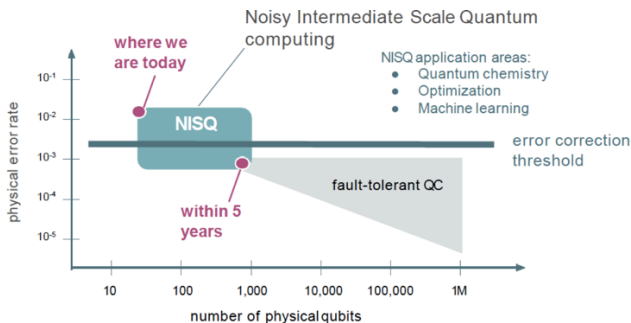
Method	Speedup	Amplitude amplification	HHL	Adiabatic	qRAM
Bayesian inference <sup>106,107</sup>	$O(\sqrt{N})$	Yes	Yes	No	No
Online perceptron <sup>108</sup>	$O(\sqrt{N})$	Yes	No	No	Optional
Least-squares fitting <sup>9</sup>	$O(\log N)^*$	Yes	Yes	No	Yes
Classical Boltzmann machine <sup>20</sup>	$O(\sqrt{N})$	Yes/No	Optional/No	No/Yes	Optional
Quantum Boltzmann machine <sup>22,61</sup>	$O(\log N)^*$	Optional/No	No	No/Yes	No
Quantum PCA <sup>11</sup>	$O(\log N)^*$	No	Yes	No	Optional
Quantum support vector machine <sup>13</sup>	$O(\log N)^*$	No	Yes	No	Yes
Quantum reinforcement learning <sup>30</sup>	$O(\sqrt{N})$	Yes	No	No	No

\*There exist important caveats that can limit the applicability of the method<sup>51</sup>.



# The NISQ era

- Current quantum computers...
  - are affected by noise and errors (not fault-tolerant)
  - have a limited number of qubits (below 1000)
  - are not fully connected
- They may prove useful in some applications

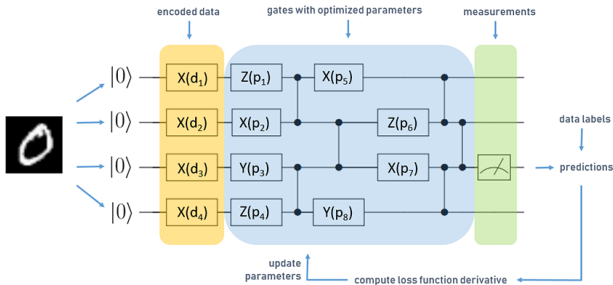


"Quantum computing in the NISQ era and beyond" Preskill, 2018 <https://arxiv.org/abs/1801.00862>

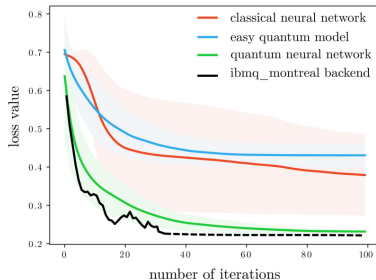
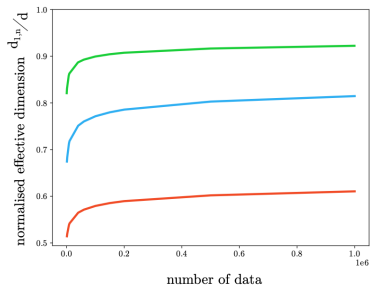
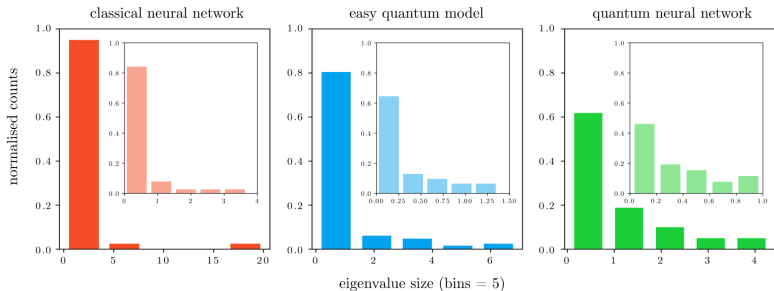


# Variational circuits and QML

- Variational circuits are one of the central techniques in QML
- They allow us to...
  - embed data
  - train parameters



# The power of Quantum Neural Networks





## Generalization in quantum machine learning from few training data

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Matthias C. Caro<sup>1,2</sup>✉, Hsin-Yuan Huang<sup>3,4</sup>, M. Cerezo<sup>5,6</sup>, Kunal Sharma<sup>7</sup>,  
Andrew Sornborger<sup>5,8</sup>, Lukasz Cincio<sup>9</sup> & Patrick J. Coles<sup>9</sup>

Modern quantum machine learning (QML) methods involve variationally optimizing a parameterized quantum circuit on a training data set, and subsequently making predictions on a testing data set (i.e., generalizing). In this work, we provide a comprehensive study of generalization performance in

### RESEARCH

#### RESEARCH ARTICLE

#### QUANTUM COMPUTING

### Quantum advantage in learning from experiments

Hsin-Yuan Huang<sup>1,2\*</sup>, Michael Broughton<sup>3</sup>, Jordan Cotler<sup>4,5</sup>, Sitan Chen<sup>6,7</sup>, Jerry Li<sup>8</sup>, Masoud Mohseni<sup>9</sup>, Hartmut Neven<sup>3</sup>, Ryan Babbush<sup>3</sup>, Richard Kueng<sup>3</sup>, John Preskill<sup>2,3,9</sup>, Jarrod R. McClean<sup>3\*</sup>

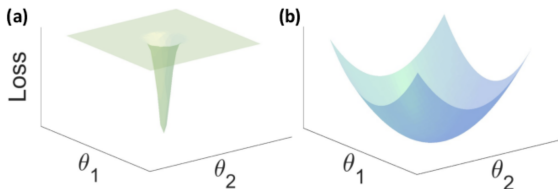
Quantum technology promises to revolutionize how we learn about the physical world. An experiment that processes quantum data with a quantum computer could have substantial advantages over conventional experiments in which quantum states are measured and outcomes are processed with a classical computer. We proved that quantum machines could learn from exponentially fewer experiments than the number required by conventional experiments. This exponential advantage is shown for predicting properties of physical systems, performing quantum principal component analysis, and learning about physical dynamics. Furthermore, the quantum resources needed for achieving an exponential advantage are quite modest in some cases. Conducting experiments with 40 superconducting qubits and 1300 quantum gates, we demonstrated that a substantial quantum advantage is possible with today's quantum processors.

quantum-enhanced experiments have a similar exponential advantage in a related scenario shown in Fig. 1C, in which the goal is to learn about a quantum process  $\mathcal{E}$  rather than a quantum state  $\rho$ . Advantages of entangling measurements over single-copy measurements have been noticed previously (11, 12), but our work goes much further by establishing an advantage that scales exponentially with system size.

Building on previous observations (8, 13), we proved that for a task that entails acquiring information about a large number of noncommuting observables, quantum-enhanced experiments could have an exponential advantage even when the measured quantum state is unentangled. Our work substantially reduces the complexity of the required quantum-enhanced experiments, improving the prospects for near-term implementation. By performing experiments with up to 40 superconducting qubits, we showed that this

# Limitations in QML

- Hardware size
  - Feature and instance selection
  - Few trainable parameters
- Noise and errors
- Device access
- Inherent problems (barren plateaus, architectures...)



# To know more...

1st Edition

## A Practical Guide to Quantum Machine Learning and Quantum Optimization

This book provides deep coverage of modern quantum algorithms, including machine learning and optimization, to help you solve real-world problems. You'll be introduced to quantum computing using a hands-on approach that requires minimal mathematical and physical knowledge to understand the logics. You'll discover many algorithms, tools, and methods to model optimization problems with QUBO and Ising formalisms and find out how to solve optimization problems with quantum annealing, QAOA, Grover Adaptive Search, and VQE. The book also shows you how to train quantum machine learning models such as quantum support vector machines, quantum neural networks, and quantum generative adversarial networks. The book takes a straightforward path to helping you learn about algorithms through chapters illustrating them with code that's ready to be run on quantum simulators and actual quantum computers. You'll also see how to utilize programming languages such as IBM's Qiskit, Xanadu's PennyLane, and D-Wave's Leap.

By the end of this book, you'll have built a solid foundation in the fundamentals of quantum computing, along with a wide variety of modern quantum algorithms and programming skills that'll enable you to start applying quantum methods to solve practical problems right away.

### WHAT YOU WILL LEARN

- Review the basics of quantum computing
- Gain a solid understanding of modern quantum algorithms
- Understand how to formulate optimization problems with QUBO
- Solve optimization problems with quantum annealing, QAOA, GAs, and VQE
- Find out how to create quantum machine learning models
- Explore how quantum support vector machines and quantum neural networks work using Qiskit and PennyLane
- Discover how to implement hybrid architectures using Qiskit and PennyLane and its PyTorch interface

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A Practical Guide to Quantum Machine Learning and Quantum Optimization

ELÍAS F. COMBARRO  
SAMUEL GONZÁLEZ-CASTILLO



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1st Edition

## A Practical Guide to Quantum Machine Learning and Quantum Optimization

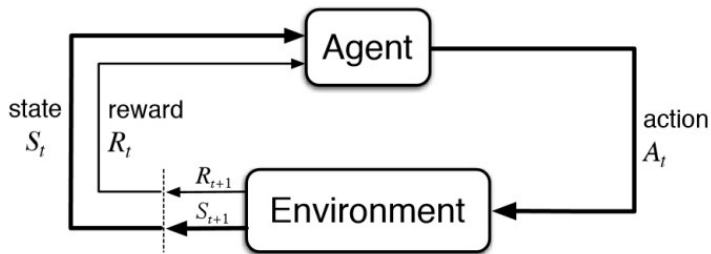
Leverage the power of quantum computing by applying quantum methods to solve practical problems

ELÍAS F. COMBARRO  
SAMUEL GONZÁLEZ-CASTILLO

Foreword by Alberto Di Meglio,  
Head of Innovation - Coordinator CERN Quantum Technology Initiative

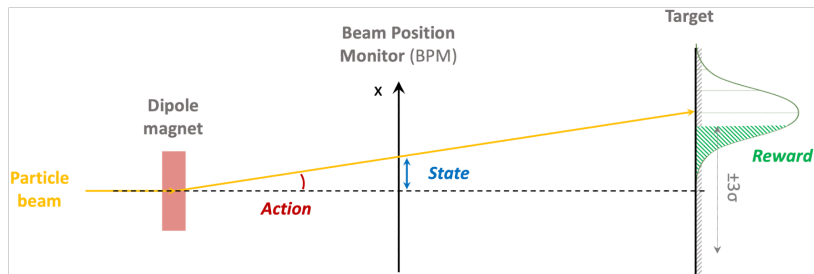


# Reinforcement learning



# Controlling particle accelerators

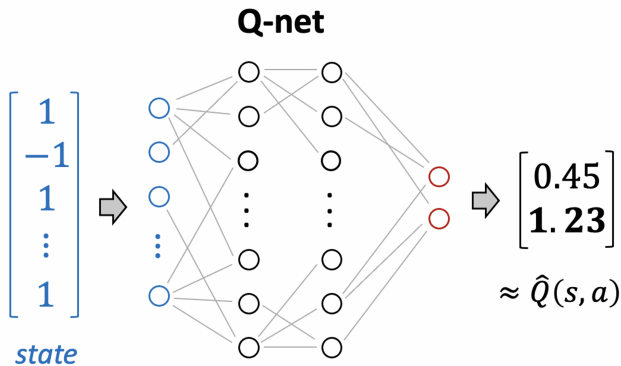
- A simple control problem at the Super Proton Synchrotron (CERN, Geneva)





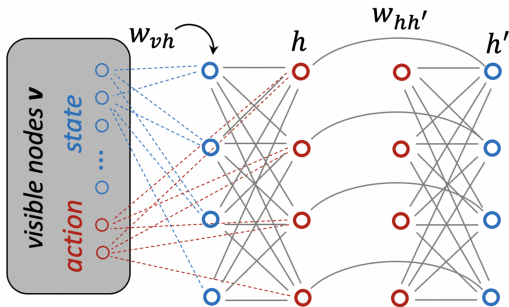
# Solving the problem with (classical) neural networks

- Feedforward dense neural network
- Two hidden layers with 8 neurons each



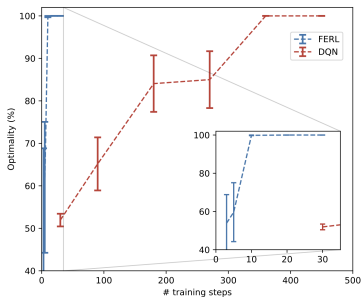
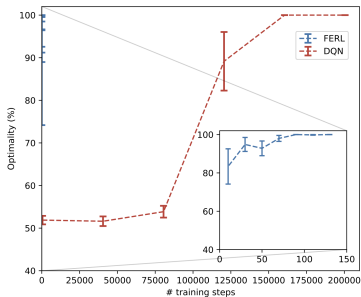
# Solving the problem with quantum Boltzmann machines

- Free energy reinforcement learning
- Quantum annealing used for energy estimation
- 16 qubits (D-Wave annealers, Chimera topology)

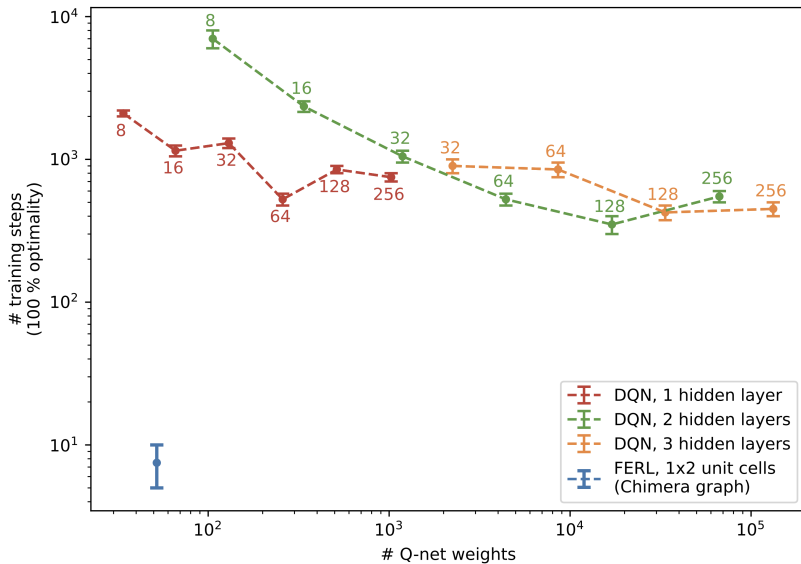


$$\hat{Q}(s, a) \approx -F(\mathbf{v}) = -\langle H_{\mathbf{v}}^{\text{eff}} \rangle - \frac{1}{\beta} \sum_{\mathbf{c}} \mathbb{P}(\mathbf{c}|\mathbf{v}) \log \mathbb{P}(\mathbf{c}|\mathbf{v})$$

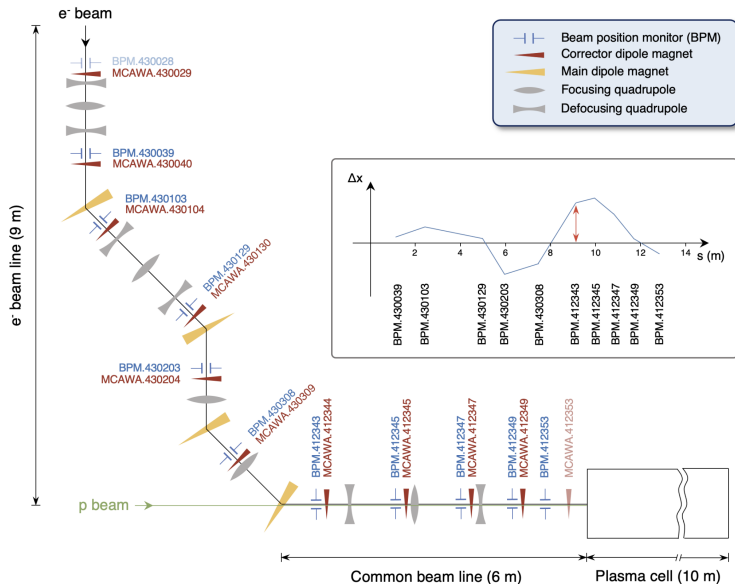
# Results with and without experience replay



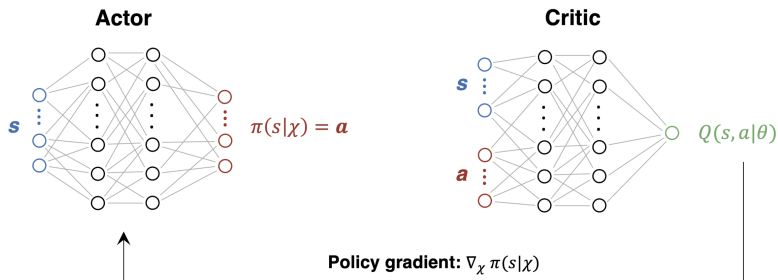
# QBM vs neural networks



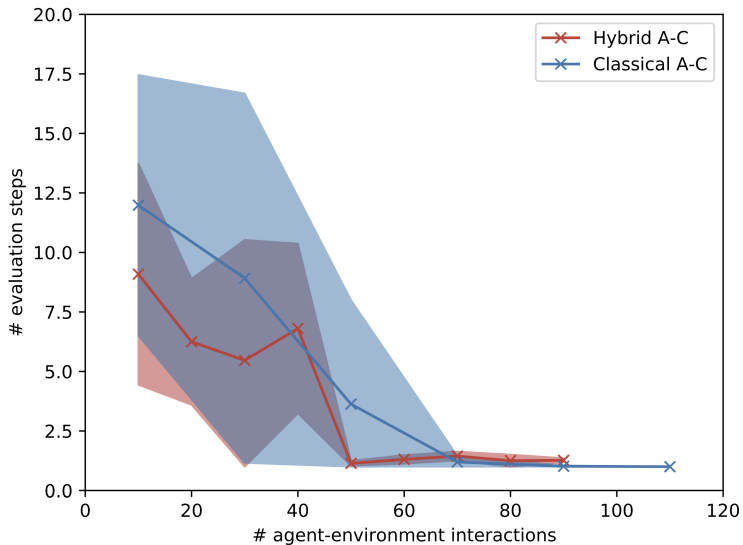
# A more complex problem



# Actor-critic architecture



# Results



## Quantum Science and Technology



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### PAPER

## Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines

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**Keywords:** energy-based reinforcement learning, quantum machine learning, accelerator physics

### Abstract

Free energy-based reinforcement learning (FERL) with clamped quantum Boltzmann machines (QBM) was shown to significantly improve the learning efficiency compared to classical Q-learning with the restriction, however, to discrete state-action space environments. In this paper, the FERL approach is extended to multi-dimensional continuous state-action space environments to open the doors for a broader range of real-world applications. First, free energy-based Q-learning is studied for discrete action spaces, but continuous state spaces and the impact of



Thank you for your attention!

