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# An Introduction to Quantum Machine Learning for Engineers

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# An Introduction to Quantum Machine Learning for Engineers

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## ABSTRACT

In the current noisy intermediate-scale quantum (NISQ) era, quantum machine learning is emerging as a dominant paradigm to program gate-based quantum computers. In quantum machine learning, the gates of a quantum circuit are parameterized, and the parameters are tuned via classical optimization based on data and on measurements of the outputs of the circuit. Parameterized quantum circuits (PQCs) can efficiently address combinatorial optimization problems, implement probabilistic generative models, and carry out inference (classification and regression). This monograph provides a self-contained introduction to quantum machine learning for an audience of engineers with a background in probability and linear algebra. It first describes the necessary background, concepts, and tools necessary to describe quantum operations and measurements. Then, it covers parameterized quantum circuits, the variational quantum eigensolver, as well as unsupervised and supervised quantum machine learning formulations.

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# 1

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## Introduction

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### Motivation

As with many engineers, I developed an early fascination for quantum theory – for its history, its counterintuitive predictions, its central role in the development of many existing technologies (semiconductors, lasers, MRI, atomic clocks) and, perhaps above all, its promise to unlock future, revolutionary, paradigms in materials, chemical, industrial, computer, and communication engineering.

At first, the topic is inviting for an engineer with my background on electrical and information engineering: The mathematical formalism is familiar, based as it is on linear algebra and probability; and concepts with wide-ranging and intriguing implications, such as superposition and entanglement, can be easily described on paper. Spend more time with it, however, and the field reveals its complexity, becoming for many, the former me included, too abstruse to invite further study. Particularly unfamiliar are ideas and architectures underlying key quantum algorithms, such as Shor’s factorization method. As if that was not enough, the impressions that most algorithmic breakthroughs are by now textbook material, and that all the “action” is currently focused on scaling hardware implementations, have kept me from engaging with the state of the art on quantum computing.

This monograph is motivated by a number of recent developments that appear to define a possible new role for researchers with an engineering profile similar to mine. First, there are now several software libraries – such as IBM’s Qiskit, Google’s Cirq, and Xanadu’s PennyLane – that make programming quantum algorithms more accessible, while also providing cloud-based access to actual quantum computers. Second, a new framework is emerging for programming quantum algorithms to be run on current quantum hardware: quantum machine learning.

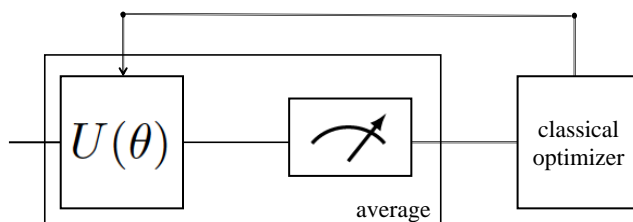
## Quantum Machine Learning

Quantum computing algorithms have been traditionally designed by hand assuming the availability of **fault-tolerant quantum processors** that can reliably support a large number of **qubits** and quantum operations, also known as **quantum gates**. A qubit is the basic unit of quantum information and computing, playing the role of a bit in classical computers. In practice, current quantum computers implement a few tens of qubits, with quantum gates that are inherently imperfect and noisy. **Quantum machine learning** refers to an emerging, alternative design paradigm that is tailored for current **noisy intermediate-scale quantum (NISQ)** computers. The approach follows a two-step methodology akin to classical machine learning. In it, one first fixes a priori a, possibly generic, parameterized architecture for the quantum gates defining a quantum algorithm, and then uses classical optimization to tune the parameters of the gates.

In more detail, as sketched in Figure 1.1, in quantum machine learning, the quantum algorithm is defined by a **quantum circuit** – denoted as  $U(\theta)$  in the figure – whose constituent quantum gates implement operations that depend on a vector  $\theta$  of free parameters. Measurements of the quantum state produced by the quantum circuit produce classical information that is fed to a classical processor, along with data. The classical optimizer produces updates to the vector  $\theta$  with the goal of minimizing some designer-specified cost function.

The quantum machine learning architecture of Figure 1.1 has a number of potential advantages over the traditional approach of handcrafting quantum algorithms assuming fault-tolerant quantum computers:

- By keeping the quantum computer in the loop, the classical optimizer can directly account for the non-idealities and limitations of quantum operations via measurements of the output of the quantum computer.
- If the parameterized quantum algorithm is sufficiently flexible and the classical optimizer sufficiently effective, the approach may automatically design well-performing quantum algorithms that would have been hard to optimize by hand via traditional formal methods.



**Figure 1.1:** Illustration of the quantum machine learning design methodology: A parameterized quantum circuit with a pre-specified architecture is optimized via its vector of parameters,  $\theta$ , by a classical optimizer based on data and measurements of its outputs. As we will see in this monograph, the operation of a parameterized quantum circuit is defined by a unitary matrix  $U(\theta)$  dependent on vector  $\theta$ . The block marked with a gauge sign represents quantum measurements, which convert quantum information produced by the quantum circuit into classical information. This conversion is inherently random, and measurement outputs are typically averaged before being fed to the classical optimizer.

Quantum machine learning, intended as the study of applications of parameterized quantum circuits, is distinct from the related topic of *quantum-aided* classical machine learning. The aim of this older line of work is to speed up classical machine learning methods by leveraging traditional quantum computing subroutines. This monograph will focus solely on quantum machine learning as illustrated in Figure 1.1.

Important open research questions in the field of quantum machine learning are discussed at the end of this text. It is my hope that

researchers who may not have otherwise contributed to these research directions would be motivated to do so upon reading these pages.

## Goal and Organization

The main goal of this monograph is to present a self-contained introduction to quantum information processing and quantum machine learning for a readership of engineers with a background in linear algebra and probability. My ambition in presenting this text is to offer a resource that may allow more researchers with no prior exposure to quantum theory to contribute to the field of quantum machine learning with new ideas and methods.

The monograph is written as a textbook, with no references except at the end of each section. References are kept to a minimum, and are mostly limited to books that the reader may peruse for additional information on different topics introduced in these pages. I have also included problems at the end of each section with the main aims of reviewing some key ideas described in the text and of inviting the reader to explore topics beyond this monograph.

It may be worth emphasizing that the text is meant to be read sequentially, as I have attempted to introduce notations and concepts progressively from the first page to the last page.

The monograph does not include discussions about specific applications and use cases. There are several reasons for this. First, many applications are domain specific, pertaining fields like quantum chemistry, and are deemed to be outside the scope of this text, which focuses on concepts and tools. Second, many existing generic tasks and data sets currently used in the quantum machine learning literature are quite simplistic, and they arguably yield little insight into the potential of the technology. The reader is referred to research papers, appearing on a daily basis on repositories like arXiv, for up-to-date results, including new benchmarks and experiments.

The rest of the monograph is organized as follows:

- **Section 2. Classical bit (cbit) and quantum bit (qubit):**  
This section introduces the concept of qubit through an algebraic

generalization of random classical bits (cbits). A qubit can evolve in quantum systems via reversible linear (unitary) transformations – also known as quantum gates – or via measurements. The mathematical formalism underlying the description of both quantum gates and measurements is also covered in the section. Finally, the section illustrates a key difference in the behavior of random cbits and qubits, namely the phenomenon of interference.

- **Section 3. Classical bits (cbits) and quantum bits (qubits):** This section extends the concepts introduced in the previous section, including quantum gates and measurements, to systems comprising multiple qubits. The new phenomenon of entanglement – a form of correlation between quantum systems with no classical counterpart – is introduced, and superdense coding is presented as an application of entanglement.
- **Section 4. Generalizing quantum measurements (Part I):** The third section presents two important generalizations of quantum measurements, namely measurements in an arbitrary basis and non-selective measurements. Decoherence, density matrices, and partial trace are also presented as concepts arising naturally from the introduction non-selective measurements.
- **Section 5. Quantum computing:** Section 4 presents a brief introduction to the traditional approach for the design of quantum algorithms in gate-based quantum computers. This presentation culminates in the description of Deutsch’s algorithm, the first example of a quantum solution that can provably improve over classical algorithms. The section also describes the no cloning theorem, which sets important constraints on the design of quantum computing algorithms.
- **Section 6. Generalizing quantum measurements (Part II):** This section presents two further extensions of quantum measurements: projective measurements and positive operator-valued measurements (POVMs). POVMs represent the most general form of quantum measurement. As an example of the application of

projective measurements, the problem of quantum error correction is briefly introduced; while unambiguous state detection is presented as technique enabled by POVMs. Observables are covered, and the section ends with a description of quantum channels as non-selective quantum measurements.

- **Section 7. Quantum machine learning:** The final section provides an introduction to quantum machine learning that builds on the material covered in the previous sections. After a description of the taxonomy of quantum machine learning methods, the concepts of parameterized quantum circuits and ansatz are introduced, along with the definition of cost functions used in quantum machine learning. These are leveraged to describe the variational quantum eigensolver (VQE), as well as unsupervised and supervised learning strategies for settings in which data are classical and processing is quantum. An outlook is also provided pointing to more advanced techniques and directions for research.



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