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Quantum Machine Learning: A tutorial

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ABSTRACT

This tutorial provides an overview of Quantum Machine Learning (QML), a relatively novel discipline that brings together concepts from Machine Learning (ML), Quantum Computing (QC) and Quantum Information (QI). The great development experienced by QC, partly due to the involvement of giant technological companies as well as the popularity and success of ML have been responsible of making QML one of the main streams for researchers working on fuzzy borders between Physics, Mathematics and Computer Science. A possible, although arguably coarse, classification of QML methods may be based on those approaches that make use of ML in a quantum experimentation environment and those others that take advantage of QC and QI to find out alternative and enhanced solutions to problems driven by data, oftentimes offering a considerable speedup and improved performances as a result of tackling problems from a complete different standpoint. Several examples will be provided to illustrate both classes of methods.

1. Introduction

The increasing availability of data sets and the need of extracting information from them has spread the use of Machine Learning (ML) in a broad variety of fields. Its sound mathematical foundations [1–3] have allowed the development of reliable applications in many different problems [4,5], not only at an academic level but also in numerous commercial applications.

Quantum Computing (QC) and Quantum information (QI) [6] have also become popular fields of research, partially due to the progresses towards a real quantum advantage, i.e., a QC-based solution within a reasonable amount of time for tasks that will be impossible to be performed by a classical computer in a human-life time; a recent but very popular paper [7] claims to have attained this milestone for the first time in the task of sampling the output of a pseudo-random quantum circuit. These quantum computers tend to be made up of a sequence of quantum-logic gates. A different QC approach comes from adiabatic QC that makes use of a network of quantum nodes to represent a given problem [8] whose solution will correspond with the ground state of the system; the strategy is to come up with a simple solution where the ground state can be easily determined and then transform the characterization of the problem slowly (adiabatically) to represent the real problem circumventing the problem of local minima, and yielding considerable speedups with respect to classical computers.

The basic element of QC is the quantum bit (qubit), that has two basic states, namely, $|0\rangle$ and $|1\rangle$. A qubit $|\Psi\rangle$ can be seen as a generalization of the classical bit, that allows the superposition of $|0\rangle$ and $|1\rangle$ in a state $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where α and β are complex coefficients. The measurement of a qubit in superposition state involves that it will collapse to one of its basic states although it is not possible to determine which one before measuring it. However, the probability of having $|0\rangle$ or $|1\rangle$ as the result of the measure is known, being $|\alpha|^2$ and $|\beta|^2$, respectively. Therefore, $|\alpha|^2 + |\beta|^2 = 1$. Operations with qubits are carried out by unitary transformations U; when U is applied to a superposition state, the result is another superposition state, obtained as the superposition of the corresponding basis vectors. This is an appealing characteristic of unitary transformations, which is called quantum parallelism because it can be employed to evaluate the different values of a function $f(x)$ for a given input x at the same time although this parallelism may not be immediately useful [6], since the direct measurement on the output generally gives only $f(x)$ for one value of x. Let $|y\rangle$ be in the superposition state $|y\rangle = \alpha|0\rangle + \beta|1\rangle$. The unitary transformation U_y may be defined as:

$$U_y : |y, 0\rangle \rightarrow |y, f(y)\rangle \tag{1}$$

where $|y, 0\rangle$ is the joint state with the first qubit in $|y\rangle$ and the second qubit in $|0\rangle$ and $|y, f(y)\rangle$ stands for the corresponding joint output state. Therefore:

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$$U_y : |y,0\rangle \rightarrow \alpha|0,f(0)\rangle + \beta|1,f(1)\rangle \quad (2)$$

that contains simultaneous information of $f(0)$ and $f(1)$, i.e., two different values of $f(x)$. This process, known as oracle or quantum black box, can process quantum superposition states with an exponential speed-up compared to classical inputs [9]. The idea can be extended to an n-qubit system:

$$|\phi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes \ldots \otimes |\Psi_n\rangle \quad (3)$$

where $\otimes$ is the tensor product. The system shown in Eq. (3) can simultaneously process 2^n states but only one of them could be accessible by means of a direct measurement.

QC and ML have converged towards a new discipline, Quantum Machine Learning (QML) [10–12], that brings together concepts from both fields to come up with enhanced solutions, either improving ML algorithms, quantum experiments, or both. In fact, two main approaches can be considered:

a) The use of quantum resources to improve ML in terms of speed-up and/or performance, obtaining alternative solutions. We can also deem here the implementation of ML algorithms in quantum computers, including adiabatic quantum annealers.
b) The use of classical ML to quantum experimentation problems, such as quantum metrology [13].

The rest of the paper is outlined as follows. Section 2 approaches ML as a field that can benefit from quantum representations, either using quantum-inspired classical ML algorithms or pure quantum versions of classical ML algorithms. Section 3 describes the use of ML to enhance quantum experimentation and metrology. This tutorial ends up in Section 4 with some conclusions and perspectives for the field in the near future.

2. Quantum approaches to Machine Learning

The benefits of applying quantum methods to learning algorithms have been widely reported in the last few years [14–25]. Although most of the initial works in this framework pursued a reduction of the computational complexity with an associated speedup, some recent works have also analyzed how quantum methods can provide alternative learning representations that may result in different solutions to those provided by classical ML, oftentimes outperforming it. Some examples include quantum clustering [21,22,26], quantum autoencoders [23], quantum Reinforcement Learning (RL) [25,27], quantum nonlinear modeling [17,28–30], or quantum speedup for active learning (AL) [31], to name a few.

A crucial topic is also the study of how different types of learning (inductive, transductive, active, supervised, unsupervised, reinforced or semi-supervised) map to quantum processes in general, and the suitability of each kind of learning to different environments. In fact, an accurate definition of learning in quantum environments is not trivial, as difficulties not present in the classical realm may arise, e.g., an entanglement between the learning agent and its environment. Therefore, it may make sense to propose radically new quantum oracles as the standard classical ones do not meet all the requirements and nuances of quantum environments.

Finally, quantum annealing (adiabatic quantum computing) also deserves some words. The number of qubits is increasing at a fast pace thus enabling more and more complex calculations and the extraction of useful knowledge [32]. Its application to learning problems [15] has also been tested successfully. However, one should also be aware of implicit imperfections; although it is possible to violate the limits imposed by the gap in the adiabatic evolution and perform the process at a temperature higher than necessary, the result might be a low-level excited state instead of the ground state; this is still very useful for ML but should be taken into account.

By way of illustration, two examples of quantum versions of ML approaches, namely, Quantum Clustering (QC) and quantum autoencoders will be shown in Sections 2.1 and 2.2.

2.1. Quantum clustering

QC is a quantum-inspired clustering approach based on the Schrödinger equation [26]; it generates a potential function $V(\mathbf{x})$ as the ground state:

$$H\Psi \equiv \left(-\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x})\right)\Psi(\mathbf{x}) = E\Psi(\mathbf{x}) \quad (4)$$

where H is the Hamiltonian, E the energy eigenvalue and Ψ the wave function. Originally, Ψ was proposed as a Parzen density estimator with a given length scale parameter, σ. Data samples are eventually allocated to clusters by applying the gradient descent over the potential function. QC shows a high sensitivity associated with the length scale, especially because it controls the shape of the Gaussian kernel usually associated with a wave function, which is employed in the Schrödinger equation with the role of a density estimator. The parameter σ is of crucial relevance as it measures the overlap between the wave function components from neighboring observations, thus having a great impact on the shape and smoothness of the resulting potential function, affecting the number of local minima and, consequently, also the final number of clusters [21,22]. The outcome of QC is an energy surface –the potential function–; the data samples are mapped onto this surface, eventually converging in clusters.

Recently, a probabilistic framework of the quantum clustering was proposed [22]. It defines a likelihood function to measure goodness-of-fit to the data, that carries out a parameter optimization without any a priori knowledge of the data structure. The proposed approach also indicates the presence of hierarchical data structure, identified by local minima. The probabilistic approach has two additional advantages. First, an assessment of the probability of cluster membership that can identify outliers. Second, the likelihood appears to be very correlated with the supervised Jaccard score, thus suggesting that the goodness of probabilistic QC can be objectively assessed despite being completely unsupervised.

2.2. Quantum autoencoders

Quantum autoencoders have been proposed in recent years, in analogy with autoencoders of standard Machine Learning, as a way to efficiently employ the resources in a quantum computation. Two proposals were made initially [33,34], in which a compression of the quantum resources needed for a specific quantum computation was suggested. Namely, if one starts with a certain Hilbert space of, say, n qubits, one figures out whether one can employ $n' < n$ qubits for the desired quantum computation. For this, the original quantum states one would like to encode in a smaller Hilbert space, are fed onto a quantum circuit with a certain, parameterized, encoding n-qubit unitary gate, followed by a quantum circuit with n' qubits, and a parameterized decoding n-qubit unitary gate. After measurement of the output quantum state, the unitary gates are optimized by tuning their parameters in order to maximize the fidelity of the output with respect to the input quantum states, repeating this quantum–classical sequence several times, until convergence. Finally, the outcome of the quantum autoencoder is the encoding unitary operation.

More recently, another version of a quantum autoencoder based on approximate quantum adders was proposed [23]. In this work,

compression of quantum information was carried out via the use of a quantum adder, which was previously optimized to add with high fidelities certain families of quantum states. In this case, the compression of the quantum information is related to the addition of the incoming quantum states, which are therefore encoded in a smaller number of qubits.

A number of quantum implementations of quantum autoencoders have been realized in experiments, including quantum photonics [35] and superconducting circuits [36].

3. Machine Learning in quantum environments

On top of quantum versions of classical ML algorithms, the other main QML approach is based on the use of classical ML algorithms in the field of quantum experimentation and quantum information. One of the first promising results was related to the application of RL to adaptive quantum metrology [37], where a RL-based control of quantum processes turned out to outperform standard greedy approaches. RL has also been applied in the field of QC for online nonconvex optimization in circuit simulations [38] and ultra-cold-atom experiments [39].

Measure control is another –relatively– popular application of RL to QC [13]. The relevance of this problem stems from the fact that the data encoded on a quantum state might be difficult to be accessed for any kind of computation. In this framework, there have been a couple of recent efforts to set AL for quantum experimentation due to its appealing characteristics in this environment, as only the most relevant labels are required thus minimizing the number of measures that make superposition states collapse [40,41].

Although ML and computational theory have already shown their usefulness in given quantum scenarios, the definition of new learning paradigms in which all the elements are quantum is still a research avenue, that can pave the way of a theory for knowledge discovery in quantum systems.

A number of works have studied the application of ML to extract information from physical systems not necessarily linked to quantum information processing. As many fields of Physics involve the acquisition of huge amounts of data, the use of ML to extract information is quite reasonable [42]. Some recent works show indeed the capability of ML to model complex physical systems with great accuracy and with the added advantage of its flexibility in contrast with the classical models applied in Physics that tend to follow a very restricted formulation [43–46]; therefore, ML may have the capability of modeling some nuances that might be present in the data but have not yet been explicitly considered in previous formulations and modeling approaches to the problems.

Within this collaborative field that brings together ML and Physics, some works have recently proposed the use of the so-called Physics-based ML [47,48], i.e., ML methods that are usually applied to Physics problems and with the appealing characteristic of being inspired in physical concepts. Although this is not something new, since classical ML methods like the Hopfield neural network [49] or Boltzmann machines [50] have a fundamental physical inspiration, the current massive use of ML techniques by physicists have boosted this kind of approaches.

Sections 3.1 and 3.2 show two particular cases of how quantum information can benefit from the use of ML, namely Quantum Reinforcement Learning (QRL) and AL as a way to minimize the loss of quantum information in the process of measuring.

3.1. Quantum Reinforcement Learning

Inside QML, the field of QRL has raised an increasing interest in recent years [11]. Here, the aim is to develop "intelligent" quantum agents, which may interact with the outer world and learn from it, in order to achieve some specified goal. In this sense, several works have made interesting proposals in the past few years [27,31,51,25,52–55]. Some of these works deal with quantum agents interacting via Grover search with a classical environment [27,31], others deal with quantum agents coupled to an oracular quantum environment, with proved quantum speedup [51], while some other results are related to possible implementations of quantum agents interacting with few-qubit quantum environments [25,52–55]. In this sense, it is remarkable an experiment of quantum reinforcement learning with quantum photonics [54], in which a speedup was demonstrated with respect to standard quantum state tomography, in the limit of a small amount of resources available.

3.2. Active learning for retrieval of quantum information

The main challenge of retrieving quantum information lies in designing a strategy to minimize the cost of measurements, while extracting the relevant information. Since AL takes into account the cost of labeling, i.e. fidelity loss caused by measurement [56], it fits well with the framework of quantum measurement in which measures are to be minimized. In particular, AL is based on labeling samples with maximal uncertainty so that a model trained on a small set of labeled samples can obtain a similar performance to that obtained when labeling all samples.

AL protocols for retrieving quantum information were recently proposed in [41] for a binary classification problem defined by extracting information from qubits through weak measurements. In particular, a quantum state in a lattice of $21 \times 21 = 441$ qubits was mapped onto a spin system with transformation $|0\rangle \rightarrow |\uparrow\rangle$ and $|1\rangle \rightarrow |\downarrow\rangle$. The achieved results show that labeling only 5% samples can lead to a 90% rate estimation.

4. Conclusions

This tutorial has presented an overview of the current status of QML, an emergent research and technological topic that brings together concepts from QI, QC and ML. The two main QML approaches, namely adding quantumness to classical ML and the use of ML to extract information from quantum systems have been described and illustrated with several examples.

Our view about the future of the field is that an effort should be made in order to come up with collaborative solutions involving ML practitioners and physicists because, as described in the tutorial, most of the progresses so far have been based on analyzing either what ML can do for QC or the other way around. Nonetheless, very few attempts have been done with a unified perspective that could lead to robust definitions of quantum learning. Another result of this collaboration could be the proposal of new algorithms to efficiently analyze data while exploiting quantum properties at the same time and with the possibility to be implemented in quantum computers and/or quantum annealers.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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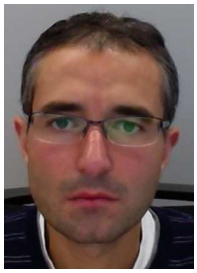

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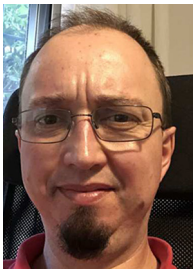

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