ESANN 2020 proceedings, European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning. Online event, 2-4 October 2020, i6doc.com publ., ISBN 978-2-87587-074-2.
Available from http://www.i6doc.com/en/.

Quantum Machine Learning

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Abstract.
Machine Learning (ML) is becoming a more and more popular field of knowledge, being a term known not only in the academic field due to its successful applications to many real-world problems. The advent of Deep Learning and Big Data in the last decade has contributed to make it even more popular. Many companies, both large ones and SMEs, have created specific departments for ML and data analysis, being in fact their main activity in many cases. This current exploitation of ML should not mislead us; while it is a mature field of knowledge, there is still room for many novel contributions, namely, a better understanding of the underlying Mathematics, proposal and tuning of algorithms suitable for new problems (e.g., Natural Language Processing), automation and optimization of the search of parameters, etc. Within this framework of new contributions to ML, Quantum Machine Learning (QML) has emerged strongly lately, speeding up ML calculations and providing alternative representations to existing approaches.

This special session includes six high-quality papers dealing with some of the most relevant aspects of QML, including analysis of learning in quantum computing and quantum annealers, quantum versions of classical ML models –like neural networks or learning vector quantization–, and quantum learning approaches for measurement and control.

1 Introduction

Machine Learning (ML) has probably become the most usual choice to analyze data sets in order to extract useful knowledge from them. ML is well founded mathematically speaking and, hence, it can come up with robust and sound solutions to data analysis whose conclusions are supported by a strong mathematical basis [1, 2, 3]. ML applications have increased exponentially in the last decade [4, 5], not only at an academic level but also in commercial applications with more and more companies specialized or with departments devoted to this topic.

Quantum information (QI) and Quantum Computing (QC) are also very fruitful and popular fields of research [6]. Researchers have been struggling for a long time in order to achieve the so-called quantum advantage, i.e., to come up with a QC-based solution that can be obtained within a reasonable amount of

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time for problems that will be impossible to be solved by a classical computer in a human life time; the recent 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.

Adiabatic quantum computing is another approach to QC that has already shown a considerable speed-up in some instances compared to classical computational approaches thanks to its capability of finding the global optimum of a given cost function, thus circumventing the problem of local minima [8].

To have a general overview of QC, one needs to know that is driven by the quantum bits (qubits), a quantum generalization of the classical bit. The two basic states of a qubit are $|0\rangle$ and $|1\rangle$, which correspond with the states zero and one, respectively, of a classical bit. A qubit $|\Psi\rangle$ generalizes its classical counterpart because it allows states formed by the superposition of $|0\rangle$ and $|1\rangle$, namely, $|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$, 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, but there is no way to determine in advance which one; the unique available information is that the probability of $|0\rangle$ is $|\alpha|^2$ and the probability of $|1\rangle$ is $|\beta|^2$, hence, $|\alpha|^2 + |\beta|^2 = 1$. The main operation when dealing with qubits is the unitary transformation U. When U is applied to a superposition state, the result is another superposition state which is the result of superposing all 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. However, this parallelism is not 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 $|y, 0\rangle$ stands for the joint state with the first qubit in $|y\rangle$ and the second qubit in $|0\rangle$ and $|y, f(y)\rangle$ is the corresponding joint output state. Therefore:

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

that contains simultaneous information of $f(0)$ and $f(1)$, i.e., two different values of $f(z)$. This process is known as oracle or quantum black box; it 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:

$$|\phi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes \ldots \otimes |\Psi_n\rangle \tag{3}$$

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. The key aspect here is how to exploit this parallelism without destroying the superposition.

Both fields, QC and ML have lately converged towards a new discipline, Quantum Machine Learning (QML) [10], that brings together concepts from

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both fields to provide enhanced solutions, either improving ML algorithms, quantum experiments, or both. Two main approaches can be considered:

1. The use of quantum resources to improve learning, usually in terms of speed-up, but also giving alternative representations to deal with modeling and learning. We can also deem here the implementation of ML algorithms in quantum computers, including adiabatic quantum annealers.

2. The application of classical ML approaches to quantum experimentation problems, such as quantum metrology [11].

Although this special session is not the first attempt to join efforts from the fields of ML and QC, interdisciplinary collaboration is still scarce, as a matter of fact. Therefore, the organizers have tried to attract papers from relevant groups in the field in order to publish last developments, facilitate its access by other researchers and encourage networking.

The rest of the paper is outlined as follows. Section 2 presents the most common approaches within QML, including a number of relevant references. Section 3 gives an overview of the papers accepted in this special session, all of them with a high scientific quality. This tutorial ends up in Section 4 with some conclusions and perspectives for the field in the near future.

2 Quantum Machine Learning

This section aims at setting the framework of the special session by means of briefly describing some of the most popular QML approaches as a previous step to introduce the papers of the session. It can be considered that there are two main views of QML depending on the beholder; either what QC and QI can do for ML (Section 2.1) or the relevance of ML in quantum experimentation (Section 2.2).

2.1 A quantum insight of Machine Learning

Many scientific works have explored the the benefits of applying quantum methods to learning algorithms in the last few years [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23]. Although the main goal has been the reduction of the computational complexity, many works have also focused on the possibility of coming up with alternative data representations and novel approaches to tackle problems that result in different solutions to those provided by classical ML, usually outperforming the latter. Some examples include quantum Reinforcement Learning (RL) [23, 24], quantum nonlinear modeling [15, 25, 26, 27], quantum clustering [19, 20, 28], quantum speed-up for active learning [29] or quantum autoencoders [21], to name a few.

A very relevant topic is also the analysis of how the 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. The aforementioned references deal

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with supervised, unsupervised and reinforced approaches. Actually, an accurate definition of learning in quantum environments is not trivial, as difficulties not present in the classical realm may arise, e.g., a learning agent being entangled with the environment while the main assumption in the classical case is that they are independent of each other. It may make sense to propose new quantum oracles as the widely studied standard classical ones do not meet all the requirements and nuances of quantum environments.

Finally, it is also worth mentioning quantum annealing (adiabatic quantum computing). The fact of increasing the number of qubits is obviously allowing more complex calculations involving relevant knowledge discovery [30]. Its application in learning problems [13] 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 the ground state; this is still very useful for ML but should be taken into account.

2.2 Machine Learning for Quantum Information and experimentation

Classical ML algorithms can be applied to problems in the field of quantum information. This is a topic whose interest has increased considerably recently. One of the first promising results is related to the application of RL to adaptive quantum metrology [31], where a RL-based control of quantum processes outperforms standard greedy approaches. RL has also been applied in the field of QC for online nonconvex optimization in circuit simulations [32] and ultra-cold-atom experiments [33].

Another application of RL in QC involved measure control [11]. In fact, this is a topic of paramount relevance because the data encoded on a quantum state might be difficult to access in order to carry out any kind of computation; therefore, addressing this issue may be very helpful in order to generalize classical results to the quantum realm. In this framework, there have been a couple of recent efforts to set active learning 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 [34, 35].

How close one can get to the theoretical bounds using classical ML algorithms for quantum processes is an area that still needs more exploration. Although ML and computational theory has already shown its usefulness in given quantum scenarios, the definition of new learning paradigms in which all the elements are quantum is a promising research avenue, that can set the foundations of a theory for knowledge discovery in quantum systems.

Related to that is the fact of applying ML to extract information from physical systems (classical and quantum) not necessarily linked to quantum information processing. Many fields of Physics involve the acquisition of huge amounts of data that can be smartly analyzed by ML methods [36]. 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 [37, 38, 39, 40]; therefore, ML may have the capability of including in its 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 [41, 42], 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 [43] or Boltzmann machines [44] have a fundamental physical inspiration, the current massive use of ML techniques by physicists have boosted this kind of approaches.

3 Contributions to the 28^{th} ESANN special session on Quantum Machine Learning

Six contributions were accepted to be part of the special session "Quantum Machine Learning" at ESANN 2020. The top level of all those contributions should be stressed, given the low acceptance ratio of the conference. The accepted papers are related to the different approaches described in previous sections, and are summarily described next.

3.1 Learning algorithms

Although all the papers deal with learning one way or another, two of them are especially focused on learning algorithms. An analysis of training Boltzmann machines from the point of view of statistical physics' is presented in [45]. In particular, the authors show the unsuitability of training models in spin-glass regime and propose an alternative method to train spin models without an extensive sampling; this is illustrated by studying the effects of initializing Boltmann machines in a simple sampling regime with successful results although the frustration control may also involve some setbacks in training methods based on Gibbs sampling.

A quantum-inspired version of the well-known Generalized Learning Vector Quantization (GLVQ) is proposed in [46]. It starts by transforming the main elements of GLVQ, namely, data and prototypes, into quantum bit vectors with n dimensions defined in the corresponding Hilbert space $\mathcal{H}_n$ whose properties restrict prototype updates to unitary transformations; the resulting model is called Quantum GLVQ (QuGLVQ). The non-linear transformation shows obvious mathematical equivalence to kernel approaches in topological sense. The good results achieved in different data sets encourage a deeper analysis of the algorithm maybe including entanglement of qubits.

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3.2 Control and measurement

Two of the papers of the session deal with a topic commonly addressed in quantum systems, which is control and measurement. One of the papers [47] faces the complicated task of setting a framework to relate classical and quantum realms in terms of learning and control. The framework is then applied to a quantum adaptive phase estimation problem that is characterized by supervised learning making use of both classical and quantum control theories in unison. The main contribution of this paper is to bring together both classical and quantum control aspects in a unified quantum learning environment.

Quantum Convolutional Neural Networks (QCNN) for image recognition are analyzed in [48]. In spite of the architecture restrictions imposed by Noisy Intermediate-Scale Quantum (NISQ) computers, the achieved results are very accurate and encourage carrying on this line of research. The intermediate measures to reduce dimensionality deserve a deeper research, as an appropriate choice will likely enhance the performance of QCNN.

3.3 Learning in quantum computers

QC is a fascinating field for the intellectual challenges to overcome from the scientific and technological point of view. On top of that, the big bet in this topic by some of the most relevant technological companies of the world has increased even more its popularity, appearing even in generic newspapers, radio stations or TV channels, thus making QC a common conversation topic not only for scientists and engineers but also for anyone with some scientific and technological inquisitiveness.

Two papers of the session are related to QC. A quantum algorithm that implements a classical perceptron neuron is presented in [49]. The algorithm, tested in an IBM quantum computer, is able to carry out simple tasks related to classification and image recognition. The authors claim that the approach can be extended from a single neuron to a Multilayer Perceptron whose higher modeling capability could set the basis to run quantum artificial intelligence models in current NISQ computers. As the approach presented here still has some classical parts, a hybrid classical-quantum approach could be the most convenient solution making use both of traditional hardware and quantum computers. Nonetheless, running the network in a fully quantum coherent way would lead to the possibility of setting the network in a superposition state for different parameters of its neurons thus paving the way for using quantum algorithms in the training of neural networks.

The interesting topic of archetypes is addressed in [50], i.e., those data points that can represent the whole data set thus providing a useful knowledge and interpretability of the faced problem. The authors implement the method to obtain archetypes and allocate data points in a D-Wave's 2000Q Quantum Annealer, obtaining similar results to those that can be obtained using classical methods. The research is still in progress with a number of issues still to be addressed.

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4 Conclusions

This tutorial has presented an overview of the current state of QML, an emergent research and technological topic that brings together concepts from QI, QC and ML. The contributions to the special session are briefly described; they are relevant and novel works carried out by authors that have undoubtedly something to say in this field. The great development experienced by QC, partly due to the involvement of giant technological companies and 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.

We reckon that future research should entail a joint collaborative work between ML practitioners and physicists because most of the progresses so far have been based on analyzing either what ML can do for QC and QI or how quantum approaches can enhance ML algorithms. However, 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 or quantum annealers.

Acknowledgment

We acknowledge the funding from PGC2018-095113-B-I00 (MCIU/AEI/FEDER, UE).

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