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Physics and Machine Learning: Emerging Paradigms

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Abstract.
Current research in Machine Learning (ML) combines the study of variations on well-established methods with cutting-edge breakthroughs based on completely new approaches. Among the latter, emerging paradigms from Physics have taken special relevance in recent years. Although still in its initial stages, Quantum Machine Learning (QML) shows promising ways to speed up some of the costly ML calculations with a similar or even better performance than existing approaches. Two additional advantages are related to the intrinsic probabilistic approach of QML, since quantum states are genuinely probabilistic, and to the capability of finding the global optimum of a given cost function by means of adiabatic quantum optimization, thus circumventing the usual problem of local minima. Another Physics approach for ML comes from Statistical Physics and is linked to Information theory in supervised and semi-supervised learning frameworks. On the other hand, and from the perspective of Physics, ML can provide solutions by extracting knowledge from huge amounts of data, as it is common in many experiments in the field, such as those related to High Energy Physics for elementary-particle research and Observational Astronomy.

1 Introduction

ML has become indispensable for pattern discovery from large data sets. It is also the theory at the core of a larger set of data science tools known as data mining. It is a mature field with an astonishing array of practical applications in tasks related to modeling, prediction, classification, visualization and planning [1]. ML includes many robust methods that can transform raw data into structured information by means of learning algorithms [2].

It is hence not surprising that those learning algorithms are starting to find their way into applications of quantum information processing in three different ways. First, using quantum resources to perform learning is an attractive line of inquiry, with advantages ranging from quadratic or even exponential speedup, increased learning capacity, reduced sample complexity and better generalization performance; examples include quantum perceptrons, quantum neural networks, quantum deep learning, boosting training by Grover's search, adiabatic quantum annealing, and quantum support vector machines [3]. Second, from the perspective of quantum theory foundations, causal networks and their quantum generalizations, and the connection to non-locality are of paramount importance, whereas solid-state implementations of adiabatic quantum evolution are already bringing tangible benefits to ML practitioners [4]. Finally, classical ML applied in experimental Physics is also proving to be a fruitful avenue that deserves further exploration; this is an applied approach with relevance to experimental physicists. The first promising results were related to the application of ML to quantum information processing; in particular, using Reinforcement Learning (RL) to control the classical part of a quantum physics problem, e.g., using an agent-based approach to control measurement-based quantum computing [5].

Although computational learning theory and quantum information processing have already produced good results, interdisciplinary collaboration is still scarce in the ground. This special session tries to bring together researchers from both fields, with an interest in creating a collaborative research network; the session is also serving as a platform for the publication of ongoing research in this amazing and promising field.

Some specific technical goals that are still under study and can be accomplished by means of a collaboration between quantum information and learning theory are the following:

1. To generalize sample and model complexity measures to the quantum case; consider mixed classical-quantum complexity measures; understand the limits and trade-offs attainable by quantum resources and derive a quantum "no free lunch" theorem.

2. To establish theoretical guarantees of optimization by quantum resources when applied to learning problems; analyze generalization performance; and develop operational QML algorithms.

3. To devise algorithms and protocols for blind quantum computation in relation to QML.

4. To characterize the role and applicability of causal Bayesian networks in ML.

5. To characterize practical ML and RL tools in the optimization and control of quantum information processing not in the asymptotic limit.

6. To devise genuinely quantum learning protocols with no classical counterpart, benchmarking their performance in relevant quantum information processing tasks.

7. To explore quantum-like elements in symbolic systems for learning theory development.

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8. The development of models for quantum learning agents, including agents incorporating quantum (projective) simulation methodology, and their implementations.

2 Quantum Machine Learning

Recent theoretical developments hint at the benefits of applying quantum methods to learning algorithms [3, 4, 6, 7, 8, 9, 10]. To begin with, computational complexity can be reduced exponentially in some cases, whereas quadratic reduction can be observed in others [11]. Examples include quantum support vector machines, quantum nearest neighbor clustering, quantum associative memories, quantum RL [12] and several attempts to develop quantum neural networks [7, 13, 14, 15]. On a more practical side, quantum annealing (adiabatic quantum computing) is beginning to benefit from scalable implementations, and this hardware appears to be extremely efficient in certain global optimization and learning problems [4].

Although improved computational complexity and reduced training time are obviously of paramount relevance, it is also important to take into account that through nonconvex objective functions, QML algorithms become more robust to noise and outliers, which might make their generalization performance better than that achieved by many known classical algorithms. However, generalization performance is seldom studied in quantum algorithms, being this one of the potential areas in which it is possible to make substantial progresses.

Another topic that deserves attention is the study of how the different types of learning (inductive, transductive, active, supervised, unsupervised, or semi-supervised) map to quantum processes in general. One particular feature of quantum theory is that the data encoded on a quantum state might be difficult to access by the party performing computation on them. Addressing that issue will help generalizing known important classical results to the quantum case: sample and model complexity, the trade-off between complexity measures, "no free lunch" theorems, and the limits attainable by using quantum resources.

From a broad perspective, the question of what learning even means in general quantum environments (e.g. when the learning agent and the environment become entangled) is not trivial and needs to be investigated. Specifically, learning in quantum environments does not correspond to standard quantum oracle models, which, in contrast, have been extensively explored. Hence, the development of new frameworks and techniques is required, in order to establish the bounds of possible quantum improvements in learning.

Many practical questions still remain to be answered: are current proposals for QML operational? Can they be translated to a physical implementation? For example, Grover's search, a quantum algorithm for finding an element in an unordered set is quadratically faster than any classical version thereof, and is underlying many QML methods, but it is hard to implement in actual quantum systems, thus decreasing quadratic speedup due to imperfections. Quantum annealing suffers from similar problems: while it is possible to violate the time limits imposed by the gap in the adiabatic evolution and perform the process at a temperature higher than necessary, the result is likely to be a low-level excited state of the target model rather than the ground state. While this local optimum is still extremely useful for ML, the limits imposed by that methodology must be understood. By gaining insights on the trade-offs between the internal working of quantum strategies and their physical implementations, further efficient quantum-inspired classical learning algorithms might be derived. Related to this issue, the difference between thermal fluctuation and quantum fluctuation also needs special attention because in many cases quantum annealing outperforms simulated annealing; therefore, it is important to know the best methods for quantum fluctuations as well as to study the possibility of improving quantum annealing by means of a sort of feedback control.

3 Bayesian networks

As stated in the abstract, an intrinsic property of QML is its embodiment of probability theory. This makes this field a natural relative of Statistical Machine learning [16].

In this context, the quantum generalization of Bayesian networks and causal graphs are of special theoretical importance, as they relate to the foundations of quantum mechanics and nonlocality. The mathematical theory of causality, and especially the graphical models that describe causal probabilistic relationships have shown to be a very useful tool in a wide range of applications, such as statistics and ML [17]; recently, its relationship with quantum information has also been studied [18, 19].

In spite of its great recent success, Bayesian networks still offer many possibilities for further developments. Since classical networks can be associated with many different types of information processing, it is important to determine whether the addition of quantum effects in those problems might be at some point determined by a Bell inequality. A straightforward possibility is the generalization of classical causal networks to the quantum case; that would imply not only having a long-term impact in the foundations of Physics but also providing a new set of tools to understand the limitations of quantum mechanics as a resource in the processing of information. However, the latter would need a definition of causal networks that can entail quantum phenomena, thus developing new techniques to perform actual learning of quantum causal networks, e.g., extending variational algorithms beyond the existing state-of-the art, developing algorithms for statistical inference of quantum systems in arbitrary quantum causal networks and exploiting recent state-of-the art non-commutative optimization and factorization techniques.

4 Machine Learning and Quantum Information

While QML deals with quantum physical processes that aid learning, the use of classical ML algorithms to solve problems in quantum information theory is likely

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to become another cornerstone of the relationship between Physics and ML. For the time being, this line of research is yet to achieve wider acceptance, mostly due to the fact that present-day learning techniques are not adapted to the nature of quantum problems. However, there are a few promising results involving RL in adaptive quantum metrology [20]; heuristic-based RL techniques to design the quantum process tend to outperform standard greedy control techniques. There have also been some theoretical attemps of using RL in measurement-based quantum computing [5], and online nonconvex optimization in circuit simulation [21] and ultra-cold-atom experiments [22]; next steps of those algorithms might deal with decoherence or noise, always present in practical applications. Apart from applying classical ML in quantum information processing, a possible research avenue would entail taking ideas from learning theory to improve or develop new quantum strategies or protocols.

Although there are a number of proofs on how good certain quantum protocols and strategies can get in the asymptotic limit, even in the presence of noise and decoherence, RL and heuristic global optimization algorithms are important in the non-asymptotic limit, bringing these procedures closer to experimental reality. The key issue to explore is how close one can get to the theoretical bounds by using classical learning algorithms. Another exciting line of research is related to the increase of the size of the physical systems and the number of particles that can be achieved by adaptive quantum-enhanced metrology in a RL scenario.

The addition of computational learning theory to quantum scenarios has already been proven useful, but the definition of new learning schemes where all the elements involved are of a quantum nature might not only improve the quantum information processing toolbox, but also hint at a fundamental theory of knowledge acquisition in physical systems.

5 Machine Learning in experimental Physics

A maybe less exotic, but very useful connection between Physics and ML comes from the application of classsical ML to those problems in current Physics research in which huge amounts of data are acquired, so that there is a need to go beyond human inspection to automatically transform those raw data into structured information and usable knowledge [23, 24].

Obviously, this is a long-term research line with a promising outlook, since big data appear in many problems in Physics, such as High Energy Physics for elementary-particle research, Observational Astronomy or Remote Sensing of Hyperspectral Imagery, to name a few. Therefore, there exists a need for data-based knowledge extraction procedures capable of transferring knowledge to the Physics domain. In addition to the usual approach of using classical ML to those problems, a possible and exciting future avenue of research might come from the application of the approaches presented in Sections 2, 3 and 4 to data acquired in Physics problems, thus using ML approaches that are closer to Physics and which might provide a more realistic description of the problems.

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6 Contributions to the 24^{th} ESANN special session

Five contributions were accepted to be part of the special session"Physics and Machine Learning: Emerging Paradigms" at ESANN 2016. The high quality of all those contributions must be emphasized, given the low acceptance ratio of the conference.The accepted papers are related to different topics, most of them described in previous sections, and are summarily described next.

6.1 Quantum Machine Learning

The performance of Quantum Clustering (QC) when applied to non-spherically distributed data sets is studied in [25]; the work shows that QC outperforms K-Means when applied to a non-spherically distributed data set. The Jaccard score (JS) is used as performance measure; since JS can be set depending on QC parameters, local maxima can be found by tuning QC parameters, thus unveiling the underlying data structure. The paper also suggests that a straightforward improvement of the approach may well be related to the discovery of a method to obtain an appropriate number of clusters automatically. The QC algorithm introduced in [26] was applied in this study; it uses the Schrödinger probability wave function formed as a superposition of Gaussian probability functions; looking for solutions of the harmonic oscillator potential in ground energy state, those centroids in which the potential has local minima can be found, becoming the cluster prototypes.

A broad framework for describing learning agents in general quantum environments is provided in [27]. Different classical environments that allow for quantum enhancements in learning are analyzed, by contrasting environments to quantum oracles. The possibility of quantum improvements depends on the internal structure of the quantum environment; if the environments have an appropriate structure, there is an almost generic improvement in learning times in a wide range of scenarios.

6.2 Machine Learning and Quantum Information

In [20], authors show the relevance of well-designed classical ML algorithms in quantum physics problems. In particular, RL is proposed to discover the optimal sequence of actions that guarantees quantum-enhanced interferometric phase estimation up to 100 photons in a noisy environment. The study pays special attention to the scalability of calculations, using clustered computation and by vectorizing time-critical operations. The proposed algorithm shows to be robust to noise.

The way of training a quantum network of pairwise interacting qubits such that its evolution implements a target quantum algorithm into a given network subset is shown in [28]. The strategy followed in this work is inspired by supervised learning and is designed to help the physical construction of a quantum computer operating with minimal external classical control.

6.3 Machine Learning in experimental Physics

Authors in [29] present a ML challenge on High-Energy Physics, that was run in 2014 (`www.kaggle.com/c/higgs-boson`) with the participation of 1785 teams. While physicists had the opportunity to improve on the state-of-the-art using "feature engineering" based on Physics principles, this was not the determining factor in winning the challenge. Rather, the challenge revealed that the central difficulty of the problem was to develop a strategy to optimize the Approximate Median Significance objective function directly, which is a particularly challenging and novel problem. This objective function aims at increasing the power of a statistical test. The top ranking learning machines included techniques such as deep learning and gradient-tree boosting, two of the hottest topics in ML nowadays.

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