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Quantum Artificial Intelligence: A tutorial

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Abstract.
Artificial Intelligence (AI), a discipline with decades of history, is living its golden era due to striking developments that solve problems that were unthinkable just a few years ago, like generative models of text, images and video. The broad range of AI applications has also arrived to Physics, providing solutions to bottleneck situations, e.g., numerical methods that could not solve certain problems or took an extremely long time, optimization of quantum experimentation, or qubit control. Besides, Quantum Computing has become extremely popular for speeding up AI calculations, especially in the case of data-driven AI, i.e., Machine Learning (ML).

The term Quantum ML is already known and deals with learning in quantum computers or quantum annealers, quantum versions of classical ML models and different learning approaches for quantum measurement and control. Quantum AI (QAI) tries to take a step forward in order to come up with disruptive concepts, such as, human-quantum-computer interfaces, sentiment analysis in quantum computers or explainability of quantum computing calculations, to name a few.

This special session includes five high-quality papers on relevant topics, like quantum reinforcement learning, parallelization of quantum calculations, quantum feature selection and quantum vector quantization, thus capturing the richness and variability of approaches within QAI.

1 Introduction

1.1 Framework

Artificial Intelligence (AI) in general, and Machine Learning (ML) in particular, have shown their ability for successfully modeling a wide range of problems belonging to very different fields [1, 2, 3], not only at an academic level, but also reaching the commercial level. Quantum Computing (QC) has also become very popular [4], especially in the last few years, when the promise of a quantum advantage seems closer than ever, with the first paper claiming to achieve this quantum advantage in a very specific problem [5] and others studying quantum advantage from a more pragmatical point of view [6].

The elementary unit of QC is the quantum bit (qubit), a quantum generalization of the classical bit. Akin to the classical bit, a qubit also has two states, $|0\rangle$ and $|1\rangle$. However, the qubit generalizes its classical counterpart because it allows the superposition of the states $|0\rangle$ and $|1\rangle$, i.e., $|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$, where α and β are complex coefficients whose meaning is related to the probabilities of getting one of the two pure states after a quantum measurement; in particular, the probability of $|0\rangle$ is $|\alpha|^2$ and the probability of $|1\rangle$ is $|\beta|^2$, with the restriction $|\alpha|^2 + |\beta|^2 = 1$.

Both fields, QC and ML have lately converged towards a new discipline, Quantum Machine Learning (QML) [7], that brings together concepts from both fields to provide enhanced solutions, either improving ML algorithms, quantum experiments, or both. The basic hypothesis of this special session is that QML can be generalized by Quantum AI (QAI), akin to AI generalizing ML.

1.2 Quantum approaches for Artificial Intelligence

Quantum techniques have been successfully used to improve different characteristics of learning in the last decade; the most immediate benefit comes from speed-up [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20].However, this is not the only aspect of learning the can be benefited. Quantum approaches provide alternative representations of data sets, thus leading to different, potentially better, solutions. This includes quantum clustering [16, 17, 21], different quantum versions of classical AI models [11, 22, 23, 24], or quantum Reinforcement Learning (RL) [20, 25].

With respect to quantum annealers [9], the fact of increasing the number of qubits allows more complex calculations [26]. The use of ML to improve key steps of the computational process in quantum computers and quantum annealers have also been shown recently [27, 28], and it is an active field of research with the goal of circumventing adiabatic evolution efficiently.

1.3 Artificial Intelligence in quantum experimental setups

The pioneer applications of AI to the optimization of quantum experimentation dealt with circuit optimization [29, 30], quantum metrology [31], and RL-based control [32]. Related to RL-based control, there have been recent developments to carry it out in the framework of stream learning in order to extract knowledge from a continuously measured quantum system [33].In quantum environments, it is crucial to come up with a strategy to get information from quantum states without collapsing superposition states. Active Learning has already been used in binary and classification tasks, being able to capture most of the information of quantum states with a limited number of weak measures [34, 35].

Although most of the proposals mentioned so far involve ML, QAI, as a generalization of QML is making interesting progresses, for instance in quantum generalizations of Human-Computer Interactions, a very mature field in the classical realm [36]. Quantum Brain Networks integrate neurotechnology, AI and

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QC in order to develop an enhanced connectivity between the human brain and quantum computers [37, 38].

The rest of the tutorial is devoted to those aspects of the QAI that are faced in the papers of the special session, namely, optimization of quantum resources in section 2, quantum vector quantization in section 3, and quantum RL in section 4. In particular, we briefly describe the foundations of each topic before introducing the corresponding papers. We end up the paper with compiling conclusions in section 5.

2 Optimization of quantum resources

Resource optimization is of paramount relevance in any kind of computation. This importance is even higher in the case of the quantum realm due to the limitations of existing hardware and the specific characteristics of quantum measurement and QC. Two papers of this special session deal with optimization of quantum resources from different perspectives: quantum feature selection [39] and quantum forking [40].

2.1 Quantum feature selection

Feature selection (FS) is the generic term for those ML techniques whose goal is to select the most relevant characteristics of a given problem [41],.FS can maintain the performance of complicated models with much simpler versions, involving less coefficients. This has important consequences in terms of enhanced generalization capabilities, better interpretability and, of course, a lower amount of computational resources. Very recently, some works have proposed quantum versions for FS to be implemented in quantum environments [42, 43, 44]. Variance estimation is one the usual ways to build FS methods. In the ESANN 2023 special session on QAI, Poggiali et al. [39], focus on how quantum FS can be benefited from leveraging the variance; the authors propose a Hybrid Quantum Feature Selection algorithm, tested in two synthetic datasets. The proposed algorithm is based on the estimation of the variance of superposition states. The authors conclude that if the number of qubits is adequate, the algorithm successfully detects and eliminates features that are not informative.

2.2 Quantum forking

Besides an unnecessarily high number of features, another issue that affects quantum resources is the need of preparing many times the same initial quantum state in order to perform multiple tasks. AI usually requires huge datasets, and hence, encoding quantum states can be costly. Moreover, as quantum states cannot be copied nor reused once measured, alternative approaches are needed to optimize state preparation; one of the most promising approaches is the so-called quantum forking (QF) [45]; it follows a similar reasoning of forking in computer operating systems, in which the idea is to create a child process from a parent one, so that the child process can evolve independently; in QF, unitary

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processes in superposition are split, being drastically reduced the number of queries to a quantum random-access memory. In this special session, Berti comes up with a logarithmic variant to QF that performs state preparation for an initial quantum state only once for multiple tasks [40]; the proposal makes use of a few additional control qubits to compute an exponential number of tasks over the initial quantum state. The proposed technique is especially useful when the number of forks and qubits encoding the initial quantum state is high.

3 Quantum approaches for vector quantization

3.1 Standard vector quantization

Vector quantization (VQ) is one of the most prominent paradigms in ML and data compression. The aim is to represent vectorial data $\mathcal{X} \subset \mathbb{R}^n$ by a smaller set $\mathcal{W} \subset \mathbb{R}^n$ of prototype vectors $\mathbf{w}_k$ such that $|\mathcal{W}| \ll |\mathcal{W}|$ is valid for their cardinalities. Depending on the task, the prototypes are used for pure data representation or clustering in unsupervised learning, whereas in the supervised setting, one has to deal with classification or regression learning. Thereby, the data are represented by a prototype according to the nearest prototype principle (NPC) realized as a winner-takes-all (WTA) rule

$$s(\mathbf{x}) = \operatorname{argmin}_{j=1,\ldots,|\mathcal{W}|} \left(d\left(\mathbf{x}, \mathbf{w}_j\right)\right)$$

where d is a dissimilarity measure frequently chosen as the (squared) Euclidean distance. The receptive fields $R(\mathbf{w}_j) = \{\mathbf{x} \in \mathcal{X} | j = s(\mathbf{x})\}$ form a partition of the data space. For classification tasks, each prototype is responsible for a class $c(\mathbf{w}_j) \in \mathcal{C} = \{1, \ldots, C\}$ such that a data sample $\mathbf{x}$ is classified according to $c(\mathbf{x}) = c\left(\mathbf{w}_{s(\mathbf{x})}\right)$ using the WTA rule [46].Unsupervised learning of the prototypes follows several schemes: The most prominent is standard k-means or its improved variants like k-means++ or neural gas [47, 48, 49], which use stochastic gradient descent learning (SGDL) or expectation-maximization (EM) optimization. Prototype-based classification learning is based on the famous learning vector quantization (LVQ) approaches originally suggested by Kohonen [50]. Today it is based on strong mathematical foundations known as generalized LVQ (GLVQ) usually trained by SGDL [51]. NPC guaranties interpretability of vector quantizers for both unsupervised and supervised learning [46]. Further, if the squared Euclidean distance is used for training together with SGDL, prototype adaptations are by simple vector shifts in the data space. In (G)LVQ training, those vector shifts realize an attraction in case of correct classification learning and a repelling if incorrect classification occurs. This strategy is known as attraction-repulsing-scheme (ARS).

Another promising option for vector quantization, particularly in the view of quantum machine learning, are Hopfield-networks (HN) or Boltzmann machines which show relations to statistical physics and quantum systems [52, 53]. HN can be interpreted as associative memories [54] and can be used also for vector quantization [55].

3.2 Quantum vector quantization

Quantum vector quantization (QVQ) requires an appropriate encoding of the data usually realized as amplitude or basis encoding, both being used in gate-based QC [56] and adiabatic QC [57]. Coding of the data can be interpreted as quantum feature mapping of the data into the Hilbert space defined by the Bloch-sphere [58, 59, 60, 61, 62]. Hence, the WTA represents the distance in the Bloch sphere, which can be obtained via the SWAP test together with the Hadamard test [63]. The minimum search in the WTA depends on the minimum search according to the list of all available dissimilarity values for a current system state. A quantum algorithm to find a minimum is the algorithm provided by Dürr and Høyer [64, 65] which is, in fact, an extension of the often referenced Grover search [66]. However,, it should be emphasized that due to the above-mentioned quantum feature mapping, the interpretation of the QVQ algorithm with respect to the original data space maybe limited whereas within the Bloch-sphere (Hilbert space) the prototype principle and interpretation paradigms remain true [58, 60].

Unsupervised VQ can be seen as a special quadratic unconstrained binary optimization (QUBO) problem,.A QVQ approach is discussed by Engelsberger and Villmann in this special session [67]. Further, binary variables b can be transformed into spin variables s and vice versa by the relation $b = \frac{1+s}{2}$ making the Ising model mathematically equivalent to QUBO [68] as well as to the discrete HN [69], which can be applied also for unsupervised VQ.

A supervised QVQ seems to be more challenging. For the GLVQ-approach, the ARS finds difficulties according to the repelling vector shift for prototype learning in case of incorrect classification [60, 62, 70]. A promising alternative could be to adapt HN for classification, as proposed in [71, 72], and transfer these strategies to QC. HN optimization based on adiabatic QC was already proposed in [73].

4 Quantum Reinforcement Learning

4.1 Theoretical foundations

Quantum RL is the natural quantization of standard RL protocols. In the latter, a system, called agent, interacts with its outer world, the environment, in order to obtain information from it, and subsequently adapt to it, to enhance its performance. The aim of the agent is to achieve some goal, possibly in the mid or long term. Therefore, several iterations of the agent-environment interaction are usually needed, and in each of them, depending on the outcome, rewards or punishments take place, to make the agent either reinforce its behaviour, or modify it.

In the case of quantum RL, either the agent, or both the agent and the environment, are quantum systems, such that properties like entanglement and superposition will play a role. In the literature on this topic, different approaches have been pursued, such as employing Grover search algorithm to accelerate the information processing from the agent [14], or having both a quantum agent and environment in such a way that the agent aims at learning, e.g., an unknown quantum state [20, 74, 75, 76, 77, 78, 79]

4.2 Case study: Autonomous Driving

In this special session, Hickmann et al. study the possibilities and advantages of quantum enhanced Q-learning with applications to a lane change manoeuvre [80]. They analyze multiple simple RL environments by means of variational quantum circuits. The outcomes were similar to or sometimes even an enhanced version with respect to those of a simple constrained classical agent. They have also achieved promising behavior on the more difficult lane change manoeuvre task, dealing with an environment with an observation vector size twice larger than usual. In the case of the Frozen Lake environment they obtained evidence of possible quantum speedups in convergence rate.

5 Conclusions

This tutorial has presented the framework of QAI, describing the main successful approaches considered in recent literature. Special emphasis has been put on the specific topics faced in the papers accepted in the ESANN 2023 special session on QAI, namely, optimization of quantum resources, (quantum feature selection and logarithmic quantum forking), quantum vector quantization and quantum RL. It is remarkable the high-quality of all accepted papers as well as those submitted to the special session that were not eventually published due to the low acceptance ratio.

We are enthusiastic about the future of QAI, en emergent field with multiple avenues to enhance the research in the frontiers of AI and QC, and with actual possibilities of producing useful results in many real-life applications in the next few years. Therefore, we encourage the communities of AI and QC to collaborate with each other in this fascinating field of knowledge.

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