

Quantum Computing and AI

Dr. Jollanda Shara

Gjirokaster, Albania

Abstract: Lately, two novel fields are penetrating the world of technology and promise to change considerably our everyday life. The first one is quantum computing, and the second is artificial intelligence. Both of these technologies are able to transform our industries and solve complex and challenging problems.

Quantum artificial intelligence (QAI) is indicated to be the most powerful technology for the future. QAI is a methodical logic combination of these two innovative technologies: artificial intelligence (AI) and quantum computing. The use of AI algorithms and models on quantum computers, can produce satisfying results across many branches of industry and reshape their future, as well. However, the scientists have a long way to travel over for building and using fault-tolerant quantum computers. AI can overcome many practical problems related with quantum computers. The key use cases that can be accomplished by QAI include visual perception, speech recognition, decision-making, financial analysis, and language translation. Running AI models on quantum computers is more advantageous than running the same on conventional and classical computing. ([1]) The following article will explore how these two technologies, quantum computing and artificial intelligence, interact with each other influencing considerably the innovations in many fields.

Keywords: Quantum Computing, AI, QAI, QML, QCV, QNLP, QMARL, POMDP, JSS, FJSS.

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I. INTRODUCTION

Quantum computing is a contemporary field that utilizes the principles of quantum mechanics to revolutionize computation. It has the potential to profoundly impact artificial intelligence (AI). Classical computers rely on bits to process information as either 0s or 1s. Quantum computers use quantum bits or qubits, which can exist in multiple states simultaneously due to superposition and entanglement. This fundamental difference in computing architecture promises to enhance various aspects of AI, from speeding up complex computations to enabling new algorithms for machine learning and optimization tasks. [2] Artificial Intelligence (AI) can help in identifying algorithms that minimize computation times and resource needs by utilizing sophisticated search strategies. This can increase the practicality of quantum computing for real-world applications. For instance, by utilizing AI, scientists can investigate the limitless space of potential quantum gate sequences in order to maximize their efficiency and drastically reduce operational expenses. Moreover, reinforcement learning is used to control the quantum hardware, specifically in the areas of gate optimisation and qubit calibration. RL algorithms can improve the accuracy and dependability of quantum processes by iteratively fine-tuning the control parameters based on input from the system's performance. AI technologies, such as ML, DL, and RL, are essential for the advancement of quantum computing. Together, these technologies can help to fully realize the potential of quantum systems, resulting in new discoveries in many domains. [3]

Quantum Artificial Intelligence (QAI, Quantum AI) is the intersection of both technologies. It is concerned with the investigation of the feasibility and the potential of quantum computing for AI, and vice versa, AI for quantum computing. Quantum machine learning is currently the most popular application [5, 6, 7, 12]. But, quantum AI covers more subfields of AI such as quantum reasoning [8, 9, 10], quantum automated planning and scheduling (QPS), quantum natural language processing (QNLP), quantum computer vision (QCV), quantum agents and multi-agent systems (QMAS), etc. QAI is a new and fundamentally interdisciplinary research field. But, it has made a remarkable progress in the past few years. The customized QAI algorithms could be used more successfully in solving some computationally hard problems such as the combinatorial optimization in AI applications compared to classical solutions. This has been shown, in part also experimentally on real quantum computers of the current NISQ (Noisy Intermediate-Scale Quantum) era. The direct quantum or hybrid quantum-classical methods of QAI for applications in diverse domains such as manufacturing, automated driving, transport and logistics, energy management, healthcare, finance, aerospace, climate and earth sciences, and pharmaceutical and chemical industries are under investigation, as well. ([4]) It is also important to note the differences between the two technologies for better understanding of their capabilities. Some believe that quantum computing will replace artificial intelligence and become the superior technology. In reality, both of them are quite different in terms of handling tasks. Artificial intelligence acts as a

human brain that allows other technologies to perform such tasks as thinking, learning, adapting, and so on, while quantum computing is a technology that computes data in an unimaginable way but has nothing to do with its analysis, classification, interpretation, etc. It is also a known fact that quantum computing is still in the process of becoming a complete technology capable of performing as promised. Both technologies can individually work on leveling various areas such as healthcare, finance, materials science, cybersecurity, and others. [32] Modern quantum computers are notably good at scaling computational problems to operate on many parallel complex problems, theoretically solving them exponentially faster than their classical counterpart. On the contrary, artificial intelligence via machine learning along neural networks imitates human intelligence to work with data of huge scales, reveal patterns, and predict. [32] However, when combined together, they can increase their capabilities and potential to an unprecedented level. The simplest promise of these technologies is that each of them will accelerate the other, hence increasing their capabilities and allowing to solve problems that were either intractable before (drug discovery, climate modelling), may be possible before, but at a much higher cost (optimizing supply chains), or too risky (phylogenetics, cryptography). [33]

II. QUANTUM COMPUTING

Quantum computing is an ultramodern field at the intersection of computational science, physics, and engineering. While classical computers employ 1 or 0, quantum computers utilize qubits, either 1 and 0 simultaneously. This is the key difference separating classical and quantum computing. Qubits are used in quantum computing, which makes use of the properties of quantum theory to process data. These can indicate a mixture of 1 and 0, enabling the execution of numerous calculations at once. [34] The key concepts of quantum computing include superposition and entanglement of qubits. Superposition allows qubits to be in a linear combination of multiple states simultaneously, while entanglement describes the interconnection between qubits, where changing the state of one qubit immediately affects other related qubits. The core algorithms of quantum computing include quantum parallel algorithms and quantum entanglement algorithms. Quantum parallel algorithms utilize the superposition property of qubits to simultaneously process multiple possible solutions in one calculation, achieving exponential speedup in certain problems. Quantum entanglement algorithms utilize the entanglement property of qubits to achieve more efficient computation than classical algorithms in certain problems.

2. 1. **Historical Notes:** The original idea for a quantum computer is credited to Soviet mathematician Yuri Manin, in 1980 in the introduction of his book “Computable and Uncomputable”. The American physicist Paul Benioff, working at the French Centre de Physique Theorique, presented a paper in which he described a quantum mechanical model of a Turing machine in 1980, as well. One year later, Benioff and American theoretical physicist Richard Feynman delivered separate talks on quantum computing at the first Conference on the Physics of Computation at MIT. In his lecture “Simulating Physics with Computers,” Feynman added this famous comment on how simulating a quantum system needs the construction of a quantum computer: “Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy.”

Benioff and Feynman’s papers inspired many scientists in the final decades of the 20th century. So, the British theoretical physicist David Deutsch hoped that such a computer would make it possible to test the “many-worlds interpretation” of quantum physics, in which multiple universes are said to exist across space and time in parallel with our own universe. In 1985, he published a paper in the Proceedings of the Royal Society, where he advanced the idea of a quantum Turing machine (QTM). It was the first general and fully quantum model for computation. By 1992, Deutsch and the Australian mathematician Richard Jozsa found a computational problem that could be efficiently solved on a universal quantum computer with their Deutsch-Jozsa algorithm. The problem they identified cannot, it is thought, be solved efficiently on a classical computer. For this work, Deutsch is called the “father of quantum computing.”

Other researchers began developing their own quantum computer models and algorithms. One of the most famous is Shor’s algorithm. In 1994, Peter Shor, an applied mathematician at AT&T Bell Labs discovered a method for factoring large integers in polynomial time.

It is known that prime factorization takes a very long time and it demands an algorithm that grows exponentially in running time as a function of the original number’s size. The Shor’s algorithm can be used in the public key cryptography. Theoretically speaking, Shor’s algorithm can break existing encryption systems because factorization of primes can be achieved in polynomial time, which is of great interest for cryptographic specialists and not only. It can help anyone who wants to keep secure a vitally important system like email, an online bank account, or a nuclear weapons facility. Peter Shor’s “fast” quantum algorithm attacks an exponential-time problem in mathematics. But, it has some limitations. So, the key number size of public-key encryption systems like RSA continues to grow. This means that factoring time increases as well. So, more than thousands of qubits are needed to break the encryption. But, the current generation of universal quantum computers have no more than approximately 100 qubits; an encryption-breaking quantum computer would

require a million qubits. Google Quantum AI recently has announced that it plans to build a million-qubit machine by 2030. [38]

In 1996, another Bell Labs researcher, Lov Grover, presented the pioneering paper “A Fast Quantum Mechanical Algorithm for Database Search” at the ACM Symposium on the Theory of Computing. This was followed by a another lucid piece in *Physical Review Letters* called “Quantum Mechanics Helps in Searching for a Needle in a Haystack.” The advantage of Grover’s quantum database search algorithm is that it provides a quadratic speedup for one-way function problems usually accomplished by random or brute-force search. One-way function problems could require searching for an item in an unsorted or unstructured list, optimizing a bus route, or solving a classic Sudoku puzzle. In other words, Grover’s algorithm may be applied when a function is true for one input in the entire potential solution space, and false for all of the others. Estimating one by one gives little information on what the right answer might be. Instead of this, Grover’s algorithm uses qubit superposition and interference to adjust the phases of various operations, increase the amplitude of the right item, and iteratively check and remove states that are not solutions. A measurement of the final state of the quantum computation returns the right item with certainty. Grover’s algorithm works powerfully on computational problems where it is difficult to find a solution but relatively trivial to verify one. [3]

III. ARTIFICIAL INTELLIGENCE

Artificial intelligence (AI) is a subfield of computer science that models the mechanisms of intelligent human behavior (intelligence). [37]

The dreams for constructing machines which can mimic the human behavior are as ancient as civilization itself. For instance, Hesiod tells the tale of the lethal autonomous robot Talos, who protected Crete by tossing giant rocks at enemy ships since c. 700 BC . Three centuries later a group of spirit movement machines (Bhuta vahana yanta) were built to protect the relics of the Buddha, according to legend. In medieval times, it was Roger Bacon who, supposedly, created a talking bronze head which could answer queries, like Siri or Alexa,. Samuel Butler’s 1872 utopian novel “Erewhon” is one of the earliest English-language accounts of machines with human-like intelligence. They are conscious and able to self-replicate. In the 20th century, fictional illustrations of artificial intelligence are encountered in the stories of Isaac Asimov, Philip K. Dick, and William Gibson. Hollywood, as well, has produced classic films such as “2001: A Space Odyssey” (1968), “Blade Runner” (1982), and “The Terminator” (1984), to mention some of them. [38]

A.M. Turing (1912-1954), in 1950, wrote the essay “Computing Machinery and Intelligence”. In this essay, he poses the question of how to determine whether a program is intelligent or not [Turing (1950)]. He defines intelligence as the reaction of an intelligent being to certain questions. This behavior can be tested by the so-called Turing test. A subject communicates over a computer terminal with two non-visible partners, a program and a human. If the subject cannot differentiate between the human and the program, the program is called intelligent. The questions posed can originate from any domain. However, if the domain is restricted, then the test is called a restricted Turing test. A restricted domain could be, for example, a medical diagnosis or the game of chess.

The term “artificial intelligence” itself was used in the title of a conference that took place in the year 1956 at Dartmouth College in the USA. It was invented by the American computer scientist John McCarthy. During this meeting, were presented different programs that played chess and checkers, proved theorems and interpreted texts. These programs were thought to simulate human intelligent behavior. [37]

As we mentioned above, the core of AI is to mimic human cognitive processes and decision-making abilities, achieved through techniques such as machine learning, deep learning, etc. AI can be applied successfully in various fields, such as speech recognition, image recognition, natural language processing, intelligent recommendation systems, etc. [38]

Machine learning is a particularly productive subfield of AI. It is focused on using computer algorithms to build systems that autonomously learn from a given database and/or experiences. Machine learning systems learn gradually, much in the way humans are thought to learn. As AI pioneer Arthur Samuel has pointed out, its goal is to implant in machines “the ability to learn without explicitly being programmed.” Computer scientist Pedro Domingos defines “five tribes” within the subfield of machine learning: symbolists (inspired by logic and induction), connectionists (inspired by neural networks), evolutionaries (genetic development and transformation), Bayesians (statistics and probability), and analogizers (psychology and optimization). Machine learning platforms have improved medical care, facial and speech recognition, predictive analytics, warehouse management and transportation logistics, and many other workflows and tasks. [38]

Deep learning is a subfield of machine learning, which has at its core the artificial neural networks (ANN). Neural networks mimic the connections between neurons in the human brain, achieving abstraction and learning of complex data through multi-layered neural structures. [3]

The research interest on multilayer artificial neural networks (ANNs) and deep learning is increased due to their fantastic advances in speech recognition and natural language processing (NLP), computer vision and image recognition, neuromorphic computing, sustainability science, bioinformatics, and smart devices and vehicles. Deep learning is present and dominates the top machine translation engines (SYSTRAN, Google Translate, Microsoft Translator), imaging technologies (DeepFace, CheXNet, StyleGAN), environmental monitoring systems (Green Horizons, Wildbook, PAWS) and computational creativity applications (Deep Dream, MuseNet, WaveNet).

IV. QUANTUM COMPUTING FOR AI

Quantum AI uses quantum computing to enhance machine learning algorithms, to create more powerful AI models. By utilizing the computational superiority of quantum systems, Quantum AI can solve complex problems more faster and more efficiently than classical computers and achieve exciting results, exceeding their capacity. [42]

The intersection of quantum computing and AI has the capability to transform healthcare, particularly in the field of drug discovery.

For example, quantum AI could simulate molecular interactions at an atomic level. This can help the scientists to discover possible drugs much faster and more accurately than with classical methods. [39]

One powerful application of QAI is the development of working quantum algorithms for route and traffic optimization. In effect, these quantum applications compute the quickest route for each individual vehicle in a fleet and optimizes it in real time. For example, Toyota Tsusho Corp, in collaboration with Microsoft and the quantum computing firm Jij, has shown the capability of quantum routing algorithms for reducing the wait time at red lights by 20 percent. Using a D-Wave machine, Volkswagen has successfully tested quantum computer improved navigation and route optimization applications on the CARRIS public bus fleet in Lisbon, Portugal, as well. This test aimed to reduce traffic congestion and travel times during the Web-Summit technology conference. Volkswagen also developed a quantum simulation of the optimal routing of 10,000 taxis moving between the Beijing airport and the central business district 20 miles away using D-Wave technology.

Some real-time quantum applications could also be used effectively in cross-functional supply-chain management and transportation logistics. Predictive and risk analytic QAI technology will help the forecasting, management, and disruption of hazards such as adverse geopolitical events or terror attacks, stock market crashes and financial panics, utility grid overloads, anthropogenic threats (climate change, habitat destruction, overexploitation of natural resources), social unrest, and future pandemics. [40]

4.1. Quantum Machine Learning (QML)

Quantum machine learning (QML) aims to use the principles of quantum computing to perform traditional machine learning (ML) tasks [11,12].

It is an emerging field that combines quantum computing with traditional ML algorithms to improve their performance. For example, quantum computers can process and analyze vast datasets faster than classical computers which can lead to more accurate and timely predictions. This capability can be used especially in fields like finance, where AI models need to analyze market trends in real-time, or in healthcare, where they can speed up the processing of medical data leading to faster diagnoses and treatment plans.[40]

In QML, the researchers are trying to leverage the hybrid quantum-classical computation with VQAs. Their objective is to make use of gate-based near-term quantum devices to develop innovative models improving their performance. The hybrid QML approach with the use of VQAs has many substantial similarities with the training of classical neural networks (NNs), particularly in their dependence on parameterized models, gradient-based optimization techniques, and structured layers for approximating complex functions. These similarities have facilitated the development of quantum neural networks (QNNs). QNNs are widely used in both supervised and reinforcement learning.

4.2. Quantum Reinforcement Learning

Quantum reinforcement learning is a method that combines the principles of quantum computing with reinforcement learning. It aims to address the challenges faced by agents in making decisions and learning in complex environments. Reinforcement learning (RL) is a branch of machine learning where an agent learns to make decisions by interacting with an environment to maximize cumulative rewards, outside the classification of supervised and unsupervised learning. It is used in many fields like robotics and large language models. Unlike supervised learning, which relies on labeled data, RL focuses on trial-and-error learning, using feedback from actions to improve future performance. In quantum reinforcement learning, are used the properties of quantum computing for representing and processing the states and actions of the agent and environment. This can improve learning efficiency and performance. Quantum reinforcement learning has bright application future in the field of artificial intelligence, particularly in cases such as autonomous control and interaction between

agents and the environment. For example, in areas such as autonomous driving, robot control, and game intelligence, quantum reinforcement learning can help agents learn to adapt to complex environments more quickly and achieve higher levels of intelligent behavior. [35, 43]

Recently, some researchers are interested on quantum multi-agent reinforcement learning (QMARL) for adaptive coordination in collaborative settings for the quantum gate-based model or quantum annealing [13, 14, 15].

4. 3. Quantum Optimization

Optimization is one of the most promising applications of quantum computing in AI and beyond that involves identifying a point in a search space that minimizes or maximizes a given cost function.

Optimization problems are present in artificial intelligence and include many aspects such as logistics, supply chain management, resource allocation, path planning, parameter optimization, etc.

When dealing with complex problems, the traditional optimization algorithms may face some problems such as local optimal solutions and high computational complexity. But using quantum optimization algorithms more efficient optimization may be achieved, in some cases, due to the properties of quantum computing. The central idea of quantum optimization algorithms is to simultaneously search multiple solution spaces using the quantum parallelism and quantum search algorithms in quantum computers. Shortly, this means to find solutions of optimization problems in one computation. Common quantum optimization algorithms include quantum simulators, quantum annealing algorithms, and variational quantum eigensolvers. In the field of artificial intelligence, quantum optimization algorithms can be used for optimizing neural network parameters, improving the performance of machine learning models, solving combinatorial optimization problems, etc. [35, 43]

Quantum algorithms can optimize supply chain networks by evaluating limitless situations simultaneously to determine the most efficient routes and schedules. This ability may transform many industries such as manufacturing and logistics, where even small improvements in efficiency can result in substantial cost reductions.

Natively quantum gradient descent algorithms: It is interesting to explore optimization algorithms finding approximate solutions efficiently that are natively suited to analog quantum simulators, as they can leverage the unique properties of quantum systems to address complex optimization challenges. For instance, quantum Hamiltonian descent (QHD) exemplifies this approach by mimicking gradient-based optimization through quantum dynamics. By utilizing quantum tunneling and other quantum mechanical effects, QHD enhances the ability to escape local minima and navigate challenging optimization landscapes. Such methods highlight the potential of quantum-native algorithms to complement or outperform classical techniques in optimization, particularly in situations involving highly non-convex or high-dimensional problems. [43]

Evolutionary optimization: Evolutionary algorithms are search and optimization procedures inspired by the principles of natural selection and biological evolution. These algorithms imitate biological processes such as reproduction, mutation, crossover, and the survival of the fittest enabling, so, the evolution of populations of candidate solutions over successive generations. In contrast to conventional optimization techniques, evolutionary algorithms operate on a population of solutions rather than a single point. This can inherently facilitates parallel processing. This parallelism enables them to explore diverse regions of the search space concurrently, improving significantly their capacity to evade local optima and identify global solutions. Therefore, quantum computing is an appropriate means of improving the efficacy of evolutionary algorithms by capitalizing on its inherent parallelism and computational capacity. Quantum computers can accelerate important operations within evolutionary algorithms, including fitness evaluations, mutation, and crossover procedures, by processing superpositions of potential solutions simultaneously. [43]

4. 4. Quantum Planning and Scheduling

Quantum automated planning and scheduling (QPS) explores the integration of quantum computing into AI planning and scheduling tasks, focusing on quantum-supported planning (QP) and scheduling (QS). QP addresses tasks such as online planning, which involves real-time feedback, and offline planning, which is detached from execution.

Automated planning methods in AI can be divided into online and offline planning each with certainty or under uncertainty. Offline planning is separated from the subsequent execution of produced plans and gets no feedback about it during planning, while online planning is mixed up with a controlled action execution in a closed-loop way. [4] Under uncertainty, can arise some challenges such as partially observable Markov decision processes (POMDPs) which require complex strategies like conditional plans or utility-maximizing policies. These problems are computationally expensive, with tasks often being PSPACE-complete or worse. Initial quantum methods, such as quantum POMDP models and quantum Markov decision processes (QMDPs), suggest theoretical frameworks but they have not concrete experimental validation.

In [36], is proposed a quantum-supported method for optimal path planning in robot navigation that uses Grover's quantum search in a classical tree-search procedure.

QS tackles problems like job shop scheduling (JSS) and its flexible variants (flexible job shop scheduling - FJSS), which aim to optimize job assignments on multi-purpose machines to minimize objectives like production makespan. Quantum approaches, including quantum genetic algorithms, quantum particle swarm optimization, and hybrid MILP-QUBO (mixed-integer linear programming with quadratic unconstrained binary optimization problem formulation) methods, exhibit possible speedups in special cases, such as solving scheduling tasks for up to few hundred machines and jobs. Additionally, problems like bin packing have been addressed using quantum annealing, though current hardware limitations constrain their effectiveness. ([43])

In [16], the authors suggest an iterative quantum supported hybrid MILP (Mixed Integer Linear Programming)-based optimal solution of the JSS problem which is decomposed in a way that is suitable for hybrid quantum-classical computing. Multi-agent reinforcement learning (MARL) is one classical solution approach for FJSS with dynamic changes of optimization conditions and configurations [17,18]. Now, there are only very few primary, workable approaches of quantum-supported MARL (QMARL) for this specific problem class [13], but they do not contain any experimental analysis and concrete insights on their benefits compared to the classical counterparts. (see [4])

4. 5. Quantum Computer Vision

The research on quantum computer vision (QCV) is concentrating on the investigation of the feasibility and benefits of quantum-supported computer vision methods for the perception of intelligent agents in AI. The QCV subfield of QAI is formed in the early 2000s [20]. Recently, it is noticed a revitalized research interest on advances in quantum image processing which requires the representation and processing of a given digital image on a quantum computer, and the final conversion of the processed quantum image. For example, in [19], are analyzed several variations of a quantum hybrid vision transformer for solving an image classification problem in high-energy physics the result of which is an equal performance compared to classical counterparts with a similar number of model parameters. [4]

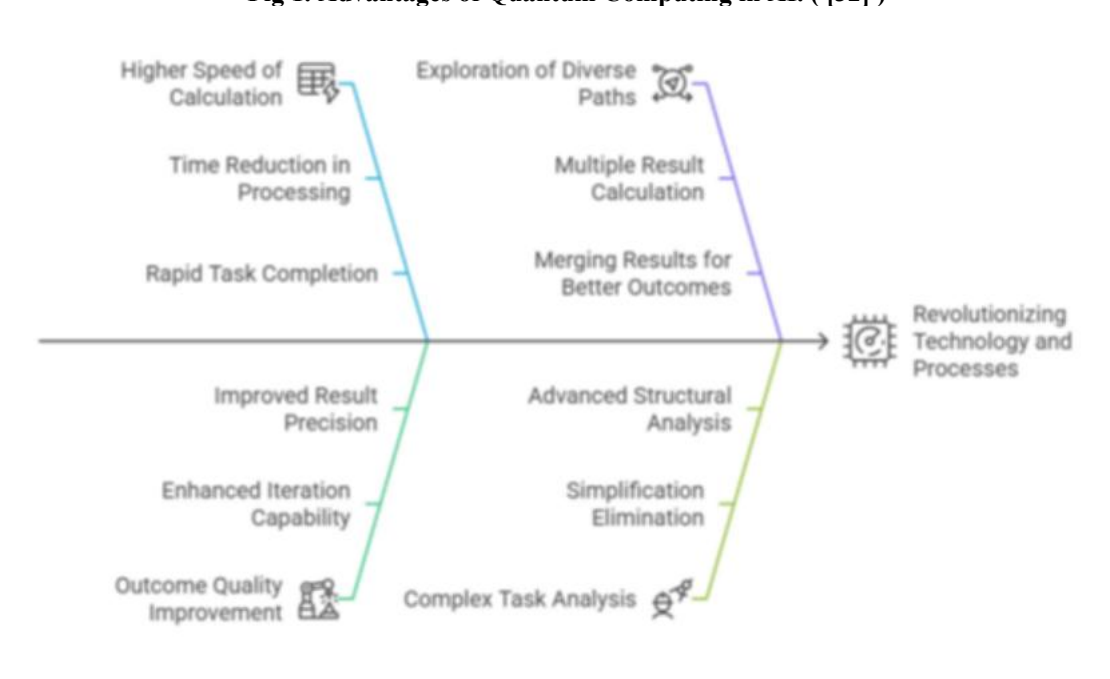
4. 6. Quantum Natural Language Processing

Quantum natural language processing (QNLP) is concerned with the representation and processing of natural language with quantum computational means. But, the utilization of NLP means for quantum computing tasks continue to be a fully unexplored direction. Most QNLP works use quantum superposition to model uncertainties and ambiguity in language or entanglement to describe both composition and distribution of syntax and semantics effectively. (see [21]) As it is shown in [22], QNLP is not simply the quantum counterpart of NLP. It allows the combination of linguistic structure and semantics or meanings in one quantum computational system, as well. Really, it represents this kind of knowledge in respectively composed variational quantum circuits, giving more effective results than those obtained in the classical case. [4]

4. 7. Data Security and Privacy

AI systems are becoming now more and more integrated into critical operations. In this situation, robust security measures are needed. Quantum technology offers innovative advancements in encryption and cybersecurity. Quantum encryption methods, such as quantum key distribution (QKD), are theoretically unbreakable, providing unparalleled security for sensitive data.

Additionally, quantum computing introduces new cryptographic protocols that could improve privacy in AI computations. For example, blind quantum computing allows a quantum server to perform computations without accessing the client's input data, output data, or even the nature of the computation itself. This level of security is vital for industries like finance, healthcare, and government where highly sensitive information is processed. [40]

Fig 1. Advantages of Quantum Computing in AI. ([32])

V. AI FOR QUANTUM COMPUTING

In this section, we are concentrating on the other direction of QAI, namely, the use of AI for quantum computing. Effective AI for quantum development requires new tools that encourage multidisciplinary collaboration, are highly optimized for each quantum computing task, and take full advantage of the hybrid compute capabilities available within a quantum accelerated supercomputing infrastructure.

NVIDIA is developing hardware and software tools that will enable AI for quantum at scales necessary to realize practical quantum accelerated supercomputing. [41]

5. 1. Quantum Algorithms and Experiment Design

Actually, there are not enough approaches for using ML methods to support both the experiment design and protocol development. Most approaches to experiment design recommend the use of reinforcement learning and reducing the influence of the human developer. For example, in [30] is suggested the use of ML methods for finding new experimental methods to create and handle complex quantum states. The author creates experiments with optical components, arranges them randomly, calculates and analyzes quantum states, and simplifies configurations based on user defined criteria, if the desired properties are met. In this work are generated correct and useful asymmetric techniques but they are not understandable intuitively. In another work, the authors have analyzed SHAP in the form of quantum Shapley (QShap) values for estimating the impact of single or group of quantum gates on PQCs, analogous with the evaluation of feature importance in classical ML. ([23]). QShap values are model-agnostic within quantum domains, treating gates as players in a coalition game to measure their contribution to tasks like expressibility, entanglement capability, or classification quality (see also [24]).

5. 2. Near-Optimal PQC Parameter Search

With warm-starting of quantum algorithms we mean the process of finding near-optimal parameters of PQCs in hybrid quantum-classical algorithms without executing them. Their objective is to minimize the number of quantum circuit evaluations required during the optimization. Classical warm-starting protocols try to relax the problem which have to be solved classically to find a good initial state [25]. In [31], the authors have investigated the integration of graph neural networks (GNNs) with QAOA to improve the parameter initialization. Various GNN architectures such as graph convolutional networks, graph attention networks, graph isomorphism networks, and GraphSAGE are explored, for example, in [31]. Experimental evaluation with benchmarks for their performance in initializing QAOA showed that all GNNs provided a more stable and safe initialization compared to random initialization. One of the advantages of GNN-based initialization is that they are capable to generalize across different graph sizes. This means that a GNN trained on smaller graph instances can still perform well on larger instances, providing a flexible and efficient warm-starting mechanism for QAOA. [4]

5.3. Transpilation of Quantum Circuits

Some challenges of NISQ devices are the low fidelity and short coherence times. Because of this, quantum circuits must be designed with minimal gates. IBM Qiskit [26] divides the quantum circuit transpilation process into six stages: Init (prepares the circuit by unrolling instructions and validating them), layout (maps virtual to physical qubits considering connectivity and calibration), routing (ensures backend compatibility with additional gates), translation (converts gates to the backend's basis set), optimization (reduces circuit complexity), and scheduling (applies hardware-aware scheduling). Actually, ML-based algorithms are utilized for most of the steps to find optimal transpiled circuits. These include evolutionary algorithms, deep neural networks, and RL methods.

5.4. Quantum Error Correction and Mitigation

Quantum algorithms are known to typically output probability distributions over possible measurement outcomes. These distributions encode the solutions to computational problems, such as optimization, simulation, or factorization. However, due to inherent hardware limitations, noise, and decoherence, the observed probability distributions often deviate significantly from their ideal counterparts. This discrepancy poses a major challenge for practical quantum computation, particularly in the current era of NISQ devices. From a computational perspective, errors in quantum probability distributions emerge due to several factors. These include gate imperfections, state preparation and measurement errors, and decoherence caused by the environment. These errors distort the statistical properties of quantum algorithms, resulting in unreliable outputs. Unlike classical errors, which can often be corrected deterministically through redundancy, quantum errors require sophisticated mitigation techniques due to the no-cloning theorem and the fragility of quantum states. The error correction actively corrects errors during the execution of a quantum circuit. In [27], is suggested a ML algorithm for continuous quantum error correction. This approach facilitates recurrent neural networks to identify bit-flip errors in continuous noisy syndrome measurements. [43]

The error mitigation is a classical post-processing step which targets the readout error. Quantum error mitigation needs a large number of circuits that have to be run in advance. Basically, each possible bitstring has to be tested for read-out errors. To improve quantum error mitigation by predicting near noise-free values from noisy quantum output the authors in [28] have trained ML models which can mitigate errors without additional circuits. reducing overhead compared to zero-noise extrapolation. [4]

5.5. Automated Control and Calibration of Quantum Computing Devices

Both quantum technologies and fundamental experiments rely on the precise manipulation and fabrication of a large number of quantum degrees of freedom. Common challenges are the efficient characterization, avoidance of inevitable hardware imperfections, and optimization of control strategies. As the qubit numbers grow and the applications become manifold, automation becomes essential and machine learning tools have been shown to be powerful for this purpose. For example, in the fully automated tuning of quantum-dot devices, the automated optimization of entangling operations on a superconducting quantum processor could substantially improve their quality, which is crucial for near-term applications. The calibration and design of quantum computing devices such as superconducting or ion trap gate-based quantum computers, quantum annealers and quantum sensors can benefit from classical ML. This is originally an application of the field of quantum optimal control theory [29]. Its goal is to find the right analogue controls for given hardware to perform desired quantum tasks. [4] ML will accelerate the process of quantum state preparation, gate operations, and measurement, leading to faster and more efficient quantum computation or quantum communication protocols on given hardware. Thus, the ML toolbox can be employed to extend the applicability of quantum devices to problems with many noisy parameters such as imaging, radar, or gravitational wave detection. ML methods can readily be utilised to characterize noise sources. By facilitating the exploration of large parameter spaces, ML can also be used to design optimized experimental setups for specific quantum tasks, such as quantum communication or quantum computing. (see [43])

Optimal control is a crucial aspect of operating a quantum processor. It ensures that all necessary operations are performed on the qubits in such a way that minimizes any noise. AI is an important tool for determining optimal control sequences that produce the most quality results possible from a quantum processor.

Foundational work presented in “Speedup for Quantum Optimal Control from Automatic Differentiation Based on Graphics Processing Units” first demonstrated the utility of GPUs to accelerate automatic differentiation for quantum optimal control. This work resulted in a 19x speedup using a GPU to optimize the preparation of a 10 qubit GHZ state. This led to work presented in “Model-Free Quantum Control with Reinforcement Learning”, which explores the application of reinforcement learning to quantum optimal control problems. [41]

5. 6. Future prospects

AI in quantum computing has great perspectives, particularly in fields like hardware optimization and quantum algorithm design. AI supported quantum algorithms are capable to completely transform industries like computational modelling and cryptography, resulting in a more effective and safe digital environment. Specifically, advances in quantum cryptography will be crucial in improving cybersecurity.

AI optimized quantum devices can significantly advance fields like global logistics, economics, and medicine in addition to cryptography. For instance, AI can optimize quantum hardware for optimal performance, enabling more accurate and fast computations. The creation of hybrid algorithms, which use both classical and quantum computing systems, could result in more effective solutions that combine the best aspects of both cases. Researchers are also exploring the establishment of quantum networks, where AI may play a decisive role in the development of effective routing, node optimization, and network control mechanisms. The interplay AI - quantum can help to advance innovative applications in data sciences and computing.

VI. CONCLUSION

AI and quantum computing together play a very important role in scientific research and computational power. Together, AI's enormous dataset processing capacity and sophisticated system optimization skills and quantum computing's unmatched computational power open up new possibilities in areas like material science, quantum chemistry, and cryptography. Even though there are still obstacles to overcome, continuous developments in AI and quantum systems are opening the door for a time when quantum technologies will be broadly available, scalable, and useful. [3] With the combination of these two technologies, the benefits are immeasurable.

QAI, a nascent field, holds tremendous potential for reshaping the future of technology and driving unprecedented progress across various domains. [2]

The researchers are enthusiastic about the future of QAI which will open new horizons to their work and with great possibilities of producing useful results in many real life applications in the next few years.

For example, in [4], the authors have pointed out some new research directions and challenges of this field. According to them, "...a future direction of QAI research across all its subfields should be the investigations under what conditions and settings in concrete (industrial) use cases are direct or hybrid quantum-classical solutions feasible with what quantum utility in practice. Additionally, the appropriate and timely transition to and investigation of the feasibility and potential of actual QAI methods on future built non - NISQ devices is a challenge. That is particularly important in the context of current expectations of the economic value of QAI applications in relevant industries..."

This work briefly presents the more significant applications of quantum computing in AI and vice versa trying to describe the main successful approaches considered in recent literature. There are numerous research works on this field and the interested reader may consult them for a more detailed information.

Conflict of interest

There is no conflict to disclose.

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