

Quantum Machine Learning Approaches for High-Dimensional Optimization Problems: A Survey

Joy Iong-Zong Chen¹, Wen-Bing Wu²

¹Professor, Department of Electrical Engineering, Da-Yeh University, Taiwan.

²Yu Da University of Science and Technology, Department of Applied Intelligent Mechanical and Electrical Engineering (AIMEE), Taiwan.

Email: ¹ljchen@mail.dyu.edu.tw, ²wbw510810@ydu.edu.tw

Abstract

Recent advances in Quantum Machine Learning (QML) bring together Quantum Computing and Machine Learning with the aim of enhancing the advantages of Machine Learning to solve problems efficiently. The properties of quantum systems (superposition, entanglement, etc.) to represent multiple states of information at once, QML can potentially offer significant advantages when solving complex high-dimensional (multidimensional) computational problems. This paper reviews the current state-of-art regarding QML in general through an organized compilation and assessment of selected studies recently published in scientific literature that were found via large electronic library catalogs based on peer-reviewed sources according to algorithms used, optimization approaches employed, and areas of applied study. This review provides comparative analyses of each selected studies for purposes of identifying major trends in QML research/practice as well as opportunities for methodological improvements and challenges still existing within QML. Finally, this review presents an overview of Quantum Computing and Quantum Data Encoding Principles utilized to translate Classical Data into Quantum States as a high-level evaluation of several popular Quantum Learning Algorithms (e.g., Quantum Neural Networks, Quantum Support Machines, and Variational Quantum Circuit). The survey describes the optimization strategies such as gradient based techniques, Bayesian Optimization and evolutionary techniques being used to improve the stability of the quantum machine learning (QML) training process. Then, it provides

examples of application areas for such QML, where healthcare analytics, environmental modelling, manufacturing optimization and analysis of biologic data are included. The comparative review of the recent academic research has identified several limitations and challenges regarding the use of QML that researchers. Although QML is believed to be capable of solving complex computational problems, issues such as noise in hardware, limited numbers of qubits and scalability present significant challenges for researchers working with this type of machine learning application. Overall, it appears that this survey provides a broad overview of contemporary developments and future trends for developing high-performance quantum learning systems.

Keywords: Quantum Machine Learning, Quantum Computing, Quantum Neural Networks, Variational Quantum Circuits, Quantum Data Encoding, Artificial Intelligence.

1. Introduction

In recent years quantum computing has gained considerable attention as an area of study related to artificial intelligence / data science. Quantum computing introduces entirely new methods of performing calculations from those traditional computing platforms. Quantum machine learning (QML) is a discipline within machine learning which combines quantum computer technology with machine learning techniques to increase the potential for learning and to improve the speed at which data can be processed. With the advent of quantum algorithms and machine learning models, there is a new way to solve some of the most challenging problems associated with data analysis/optimization [1],[2],[17]. Even though Classical machine learning algorithms perform well in most areas of machine learning, such as healthcare, finance, and manufacturing, they tend to have a lot of limitations when deal with very large data sets or data sets with high dimensionalities. Therefore, when working with large data sets it can take an excessive amount of time to execute classical algorithms, because they are limited by their computational resources. Quantum computing is one possible way to overcome these restrictions, because quantum computers are capable of running many calculations simultaneously using superposition and entanglement. In certain scenarios, the properties of these quantum algorithms allow them to work on very complicated data structures and executed much faster than their classical counterparts [6],[21].

Quantum machine learning algorithms are demonstrating the results towards enhancing classification, optimization and pattern recognition tasks. Many quanta learning models,

including quantum neural networks, quantum support vector machines and variational quantum circuits have been developed, it learns the patterns of data and consist of both quantum and classical circuits. Additionally, many studies are examining hybrid quantum-classical learning models composed of both classical optimization algorithms and quantum circuits to enable researchers to take the advantages presented by quantum computing and to work around the disadvantages of existing quantum hardware. Several studies have shown that there are large amounts of research done in the area of the development of quantum machine learning techniques. Most of the studies cover numerous aspects of quantum machine learning, such as how to design algorithms, how to encode data, and where quantum machine learning is being applied. For example, there are many studies that describe the numerous quanta learning algorithms, their associated theoretical basis, and practical applications of quantum learning [1], [4]. Additionally, there are a number of studies that look at how optimizing algorithms can be utilized to improve machine learning in high dimensionality spaces [8], [9]. Although the previously mentioned studies are useful, most of the studies do not provide an overall assessment of the type of research that is being conducted and what researchers have found regarding algorithms, optimization methods, and application areas.

Additionally, use cases for successful quantum machine learning applications are available outside of academia in areas such as medical diagnostic systems, environmental modelling, predictive analytics, and optimized industrial systems. Some papers reflect on how quantum-inspired "machine learning" models may help to improve the accuracy of predictions related to climate analysis and materials science issues [15, 19]. Quantum machine learning has also been employed as part of a diagnostic process used to assist in the diagnosis of healthcare issues and/ or to optimize intelligent manufacturing systems [7, 16]. From the applications outlined above, it would be reasonable to assume that quantum machine learning will have a significant impact on intelligent data analysis in the future. This paper provides a brief overview of quantum machine learning with an emphasis on algorithms, optimization strategies, and application domains. It serves as a resource for reviewing recent developments in quantum machine learning and for analysing selected research. In addition, it compares research findings from several recent studies and highlights some of the strengths and weaknesses of currently available approaches.

2. Fundamentals of Quantum Machine Learning

Quantum machine learning incorporates both quantum computing and machine learning algorithms into a combined system that improves both output and performance. The two primary properties of quantum computing, superposition and entanglement, provide the foundation for representing and manipulating information. When integrated together, these properties give rise to many states (or outcomes) being computed by a quantum machine at the same time. Quantum machine learning is emerging as an important area of research in artificial intelligence (AI) and computational science. The basic unit of a quantum computer is the quantum bit (or qubit). Unlike classical bits, which can exist in only two states (0 or 1), a qubit can exist in the state of 0 and in the state of 1 (simultaneously). A bit that can exist in both states (superposition) allows for complex structures of information to be represented by a qubit. The mathematical representation of any qubit is described by the following equation:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad (1)$$

In which α and β are the amplitudes of probabilities and the condition is.

$$|\alpha|^2 + |\beta|^2 = 1 \quad (2)$$

This form of representing quanta offers a way of calculating quantum processing capabilities by encoding and simulating entangled states probabilistically. Another feature of quantum computing is entanglement, where two or more qubits become correlated and share information during data processing. By simulating difficult-to-perform calculations for classical systems, entangled qubits can be utilized to execute quantum circuits. Qubits can be manipulated by quantum gates (operations) to perform any calculations needed to generate new data or produce outputs. For machine learning tasks using classical data, classical data must undergo a process called quantum data encoding (also referred to as feature mapping) prior to being able to use it in quantum circuits. Quantum data encoding has been different methods of converting classical data to quantum states, with the most popular being Encoding Basis, Encoding Amplitude, and Encoding Angle. By applying these techniques, machine learning properties can be represented on quantum circuits so that they may be used for classification type or regression by machine-learning techniques [17, 21].

A general feature mapping process may be defined as

$$|\phi(x)\rangle = U(x) |0\rangle \quad (3)$$

$U(x)$ defines how classical information or data x is to be represented as a quantum object; however, current quantum processors still exhibit weaknesses in terms of the performance characteristics, such as high levels of noise, insufficient qubits to perform complex calculations and relatively short coherence time, all of which limit their usefulness in practice. As such, many of the QML models currently being developed utilize hybrid forms of quantum-classical learning systems. In these types of systems, quantum circuits operate on the data being encoded and classical computers manage the optimization and update the parameters [5], [14].

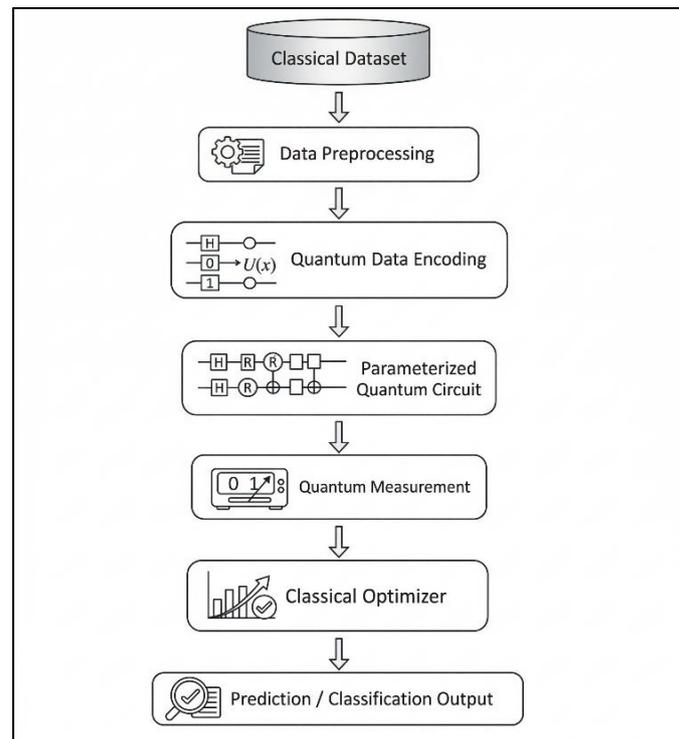


Figure 1. General Architecture of a Hybrid Quantum Machine Learning Framework

The construction of a hybrid quantum machine learning system (Figure 1) includes a generic workflow that begins with a classical data set containing training input values. Thereafter, various operations are performed on the data during the preprocessing stage, which includes cleansing and normalizing features. In the preprocessing stage, each feature is encoded into quantum states as defined by a quantum data encoding module. Once the data has been encoded, the encoded data is passed through a quantum circuit that is parameterized. The quantum circuit applies quantum gates to determine measurement results. Once the measurement results have been produced, they are sent to a classical optimizer, which reduces the loss of the circuit by adjusting the circuit parameters. Depending on the degree of

convergence achieved, cycle after cycle of measurement results and various parameters will have occurred between the quantum circuit and the optimizer. The final output of the learning process occurs when the hybrid quantum machine learning system has generated predicted or classified samples based on the learned parameters.

Initially, the data is represented using quantum methods such as amplitude encoding or using a parametric quantum algorithm consisting of quantum gates on different quanta of information. The quantum circuit is formed by using a functional form is executed against measured time-series outputs to create data structures which identify relationships among the raw data and between themselves by exploiting the properties of quantum mechanics such as superposition and entanglement. The final output of the quantum circuit, represented as a series of quantum numbers, is transformed into classical data through quantum measurements; the results of which are used to calculate a loss function representing the difference between the desired output and the actual output. Based on this loss function, the parameters of the quantum gates are altered to decrease the loss, typically using some form of classical optimization algorithm (e.g., gradient descent or evolutionary search). The loop of quantum-classical training continues for many iterations until convergence is achieved. In this process, the model is continuously refined on the optimal parameter configurations that are able to enhance the accuracy of predictions and computational efficiency.

3. Quantum Machine Learning Algorithms and Optimization Methods

A number of review articles have discussed different topics of quantum machine learning, many of these studies discuss the theoretical basis of quantum computing mostly or make their general summaries of a small number of algorithms. On the contrary, the current survey will offer structured and complete examination of the current trends of quantum machine learning through the combination of algorithmic techniques, optimization approaches, and application areas in a single framework. The survey systematically classifies the key QML models including quantum neural networks, variational quantum circuits, and quantum support vector machines as well as analyzing training and optimization methods that affect model stability and performance. Additionally, the review highlights application implementation issues that relate to near-term quantum hardware, such as the problem of noise, a small number of qubits, and scalability. This survey offers a more comprehensive view of the current developments in the research on quantum machine learning by integrating methodological

analysis and application strengths in the fields of healthcare, environmental modeling, and biological data processing, as well as establishing valuable directions in future research.

Quantum machine learning algorithms are quantum circuit-based learning algorithms that can be used to classify, regress and identify patterns. These algorithms are quantum with classical optimization algorithms that learn parameters on data. Superposition and entanglement are some quantum properties that enable models to provide complex relationships on datasets and also facilitate efficient computations within certain learning tasks [14], [21]. The Quantum Neural Network (QNN) is one of those models. QNNs rely on parameterized circuits of quantum computers which are analogous to layers of a neural network. Training is the adjustment of the circuit parameters so as to reduce the loss function. The parameters are optimized through classical optimization methods in accordance with the results of measurements. The models are used in both classification and regression tasks but may be influenced by noise and scarcity of quantum hardware [23].

The other method is the Quantum Support Vector Machine (QSVM). QSVM is the extension of classical support vector machines which relies on quantum kernel functions to project the data to the high-dimensional feature spaces. It is a quantum kernel that enables the algorithm to quantify similarity between the data points with the help of quantum circuits. QSVM applications are applied in the fields of classification and pattern recognition [24].

VQCs are also large-scale applications of QML. These circuits have trainable parameters which are optimized in the course of training. The process of training is performed with the help of a classical optimizer that modifies circuit parameters as a result of the measurement of the quantum device. The VQCs are widely applied in the hybrid quantum classical learning systems as they can run on existing noisy intermediate-scale quantum devices [14], [23].

Many of the QML models aim to reduce a loss function in their training objective. One such loss function is the common loss.

$$L(\theta) = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (4)$$

where θ is circuit parameters, y_i is the actual output, and \hat{y}_i is the estimated output.

The mathematical models that are provided in this section explain the optimization framework employed in quantum machine learning models. In QML, the learning model is usually modeled as a parameterized quantum circuit, whereby, a sequence of tuned parameters determine the quantum gates to the qubits. Such parameters define the evolution of the quantum state in the process of computation and hence directly affect the model output.

The equations that describe the transformation of the quantum state are the application of unitary operators on the coded quantum information. Measurements are then taken to the input state after it has been processed by the quantum circuit to get classical measurements that are model predictions. These predictions suggest the calculation of a loss function which measures the difference between the predicted output and the target values desired.

The loss minimization of the QML can then be defined as an optimization problem with respect to the parameters of the quantum circuit. Mathematically this process takes the form of an iterative parameter update process, where classical optimization processes are used to optimize the circuit parameters to minimize the loss. The optimization can be gradient-based (e.g. parameter-shift rules) or gradient-free (based on the circuit structure and hardware). By running the parameterized quantum circuit through many iterations of the training process, the parameterized circuit slowly reaches an optimal configuration that increases the model performance and prediction accuracy.

In this way, all equations presented characterize the process of data encoding, the transformation of a quantum circuit, the consideration of losses, and the optimization of parameters which are the main learning mechanism of the systems of quantum machine learning. Gradient-based methods, Bayesian optimization, and evolutionary algorithms are training optimization techniques that are applied with the aim of enhancing the training stability and convergence [8], [9], [12].

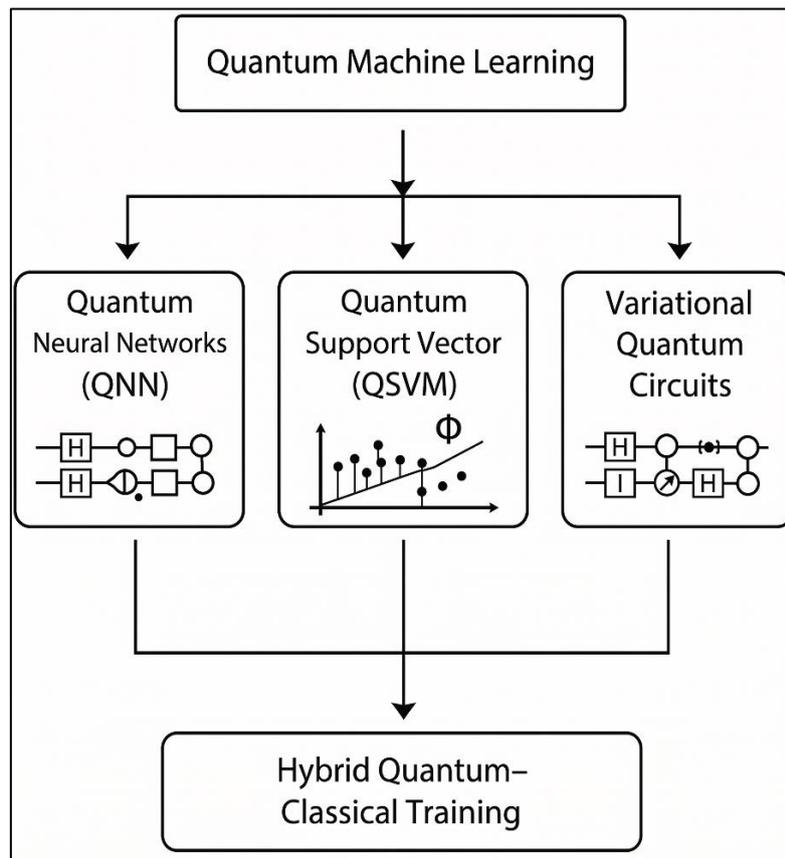


Figure 2. Main Quantum Machine Learning Algorithms

The key types of algorithms utilized in quantum machine learning are shown in Figure 2. The diagram indicates that quantum circuits are used to construct a number of learning models. Quantum neural networks refer to the parameterized circuit, which represents neural network layers and learns the parameters in the training process. The quantum support vector machine is a machine learning algorithm that utilizes quantum kernel features to project data to high-dimensional feature spaces to perform classification. Another type of significant algorithms is variational quantum circuits that consist of adjustable parameters that are trained using a classical training algorithm. The number also shows that the vast majority of practical applications are based on hybrid quantum-classical systems of learning in which quantum circuits compute and the classical optimizers update the parameters.

4. Applications of Quantum Machine Learning

There are many disciplines in Quantum Machine Learning (QML) that are related to the academic fields of research, engineering and science. These disciplines are mainly focused around improving accuracy in terms of prediction, optimising processes and providing the

capability to analyse every type of data. Due to the combination of Quantum Computing and Machine Learning, there have been many opportunities to solve problems that involve traditional algorithm development by leveraging both technologies. Many researchers are exploring the potential applications of QML to develop ways to utilise this technology in situations found in various industries [6], [10].

In the healthcare industry, there is evidence that may be found in the area of biomedical analysis (one of the largest applications for QML). With advancements in Quantum Learning, researchers will be able to analyse an unprecedented amount of complex data related to biomedical sciences and identify patterns associated with diagnoses and treatments of disease. QML has been used to predict many different types of medical outcomes, most specifically for the purposes of diagnosing hypertension and in healthcare analytics. The results of these studies have demonstrated how Quantum Algorithms may be beneficial to help the medical community make better decisions and improve prediction ability of several different areas of medicine [7], [20].

Furthermore, QML (quantum machine learning) models are useful for quantifying and predicting the changes to both the world environment and climate. Predictions of global climate and surface temperature changes, using QML models, have achieved varying levels of success compared to traditional (classical) ML models; however, in all cases, QML predictions outperformed classical ones, resulting in more accurate and efficient predictions of global climate and surface temperature changes [15]. There are also many advantages that QML has when employed in manufacturing and industrial applications. Modern industrial processes (including large-scale machinery and production systems), generate massive amounts of sensor data. That data can be analyzed with QML algorithms for failure predictions of machinery and ultimately eliminates unplanned machine down-time and its associated costs. The application of QML models for predictive maintenance significantly reduces costs associated with machine maintenance and increased productivity during the entire industrial manufacturing process [16].

The growing field of quantum machine learning (QML) offers potential applications in biological and agricultural research. Several studies have documented success in utilizing QML for the analysis of biological systems, where it has also optimized plant growth methods through the exploration of different combinations of hormones and nutrients. One example of these QML applications is simulating how hormones and nutrients interact with each other,

ultimately providing insights into the regeneration of plants. Thus, it is evident that QML provides potential solutions to challenging optimization problems in biological systems and is utilized to model complex interactions between molecular systems, as well as to identify material or chemical properties, such as the physical or chemical characteristics of materials. Several quantum model studies have also been completed for predicting molecular dynamics and polymer properties by means of quantum simulations and machine learning. The success of these applications demonstrates how effective quantum algorithms can be for simulating complex interactions among molecular entities.

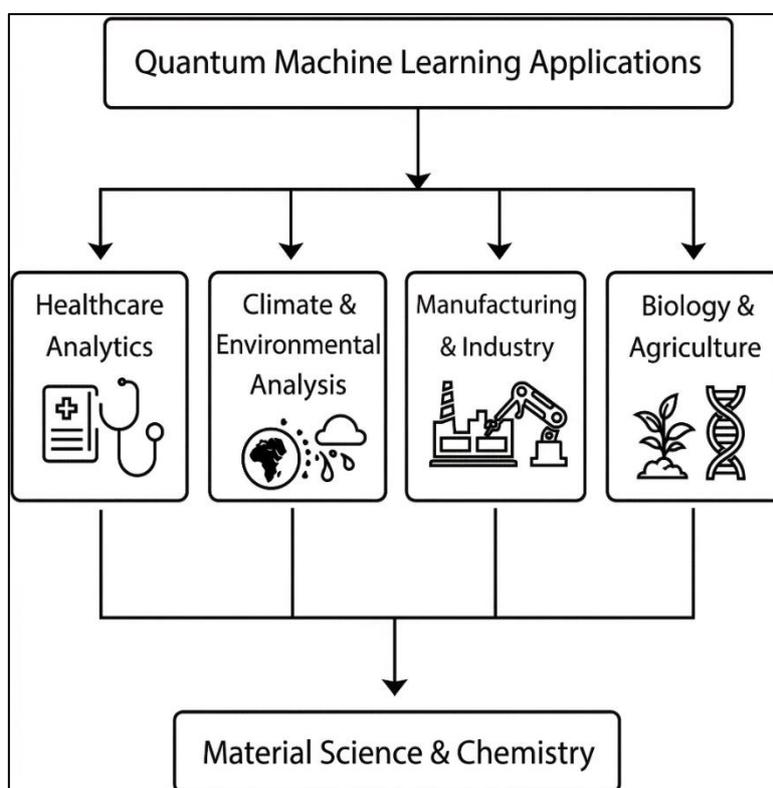


Figure 3. Application Domains of Quantum Machine Learning

The key areas of application of quantum machine learning are shown in Figure 3. The figure indicates that the QML methods are used in various fields of research that need various data analysis and optimization techniques. Quantum machine learning (QML) has become an increasingly exciting area of research, particularly with regard to applications in healthcare analytics, such as disease forecasting and medical data analytics through quantum computational models. Other areas of interest include the use of QML in predicting temperature trends and environmental patterns in climate and environmental analytics. QML's Scientific and Industrial Applications include: Manufacturing & Process Control - Predictive Maintenance & Process Improvement via Machine Learning Models with Sensor Outputs.

Biological Research & Agricultural Research - The Study of Plants & Their Interactions.
Material Science - Study of Molecular Structures & Predict Material Property using QML.
Overall, there are a number of possibilities for QML to be applied in many different types of Sci/Ind. industries. As QML and Quantum Computing technology improves there will continue to be more and more potential uses of QML to enable more complex data-driven systems.

5. Comparative Analysis of Recent Quantum Machine Learning Studies

The recent literature has discussed the various methods of enhancing the performance of quantum machine learning models. The areas largely covered in these studies are optimization strategies, application aspects and circuit design methodologies. Other publications focus on enhancing the stability of models in disturbed conditions of quantum hardware. The application of QML algorithms to real-life prediction and optimization problems is also studied in other studies. Table 1 contains a comparison of some recent studies allowing to demonstrate their areas of research, contributions, and limitations [19], [20], [21].

There are multiple pieces of research that involve optimization and the efficiency of training quantum learning models. It is suggested that noise-robust optimization methods can be used to enhance quantum circuit stability on real quantum systems [19]. Explainable models of QML model have been introduced in other studies to enhance transparency and interpretability in medical prediction systems [20]. Data encoding methods are also significant to enhance the performance of the QML models in terms of learning classical data since before processing, the classical data should be converted into quantum states [21].

In some research, QML is studied in the biological and scientific fields. To illustrate, the quantum learning models are applied to study the biological interactions and enhance optimization in the plant regeneration studies [22]. Other studies are oriented at enhancing resource use and circuit efficiency of quantum machine learning systems [23]. The use of quantum kernel algorithms can also be used in classification problems with neuron classification tasks being an example [24]. The conceptual studies also address the future and the possible contributions of QML technologies in intelligent systems [25].

Table 1. Comparison of Recent Quantum Machine Learning Studies

Ref	Method	Application	Key Contribution	Limitation
[19]	Noise-robust optimization	Polymer prediction	Improved training stability of QML circuits	Limited hardware validation
[20]	Explainable QML model	Healthcare prediction	Improved interpretability in medical diagnosis	Small dataset
[21]	Quantum data encoding analysis	QML systems	Evaluation of encoding techniques	Limited experimental testing
[22]	QML optimization framework	Plant biology	Optimization of biological growth conditions	High computational cost
[23]	Circuit optimization method	Quantum ML systems	Improved resource utilization	Scalability issues
[24]	Quantum kernel algorithm	Neuron classification	Demonstrated multiclass classification	Hardware constraints
[25]	Conceptual QML analysis	Future QML research	Identified future research directions	Lack of experimental results

Some of the recent studies, that explore optimization, applications, and algorithm development in quantum machine learning, are summarized in Table 1. The comparison reveals that there are numerous studies on enhancing the optimization of circuits and stability of training since current quantum hardware is influenced by noise and a limited number of computational resources. There is also some research on practical uses of QML in medical, biological and classifier problems. These publications indicate the increasing attention to implementation of quantum machine learning to real-world issues. Nevertheless, there are still a number of limitations. Large databases are not yet available due to which many studies are based on simulations or small datasets. Also, the scalability and the cost of computing are significant barriers to viable QML systems. Future studies must aim at enhancing hardware stability, designing efficient data encoding and coming up with scalable quantum learning models.

5.1 Limitations and Future Work

Although quantum machine learning has had favorable progress, there are a number of significant issues that prevent the practical implementation of the technology. The drawbacks of the present quantum hardware are one of the key obstacles.

- The majority of the known quantum devices work in the Noisy Intermediate-Scale Quantum (NISQ) regime, whereby quantum devices have a small number of qubits and quantum interaction mechanisms are vulnerable to noise and decoherence. These hardware limitations have a great influence on the stability and reliability of quantum learning models.
- The other significant issue is with the scalability of QML algorithms. Most of the present models are developed and trained on small quantum circuits and it is challenging to apply them to large datasets and complicated learning tasks. The higher the qubits and the depth of the circuit, the harder it becomes to preserve the coherence and therefore be able to have reliable computing.
- Data encoding is also a challenge that is critical in quantum machine learning. To convert classical data into quantum states may need sophisticated encoding methods and the cost of loading data into a quantum system may cut down on the possible computational benefits of quantum algorithms. The creation of efficient quantum feature maps and quantum encoding methods is thus still an under-researched problem.
- Parametrization of quantum circuits is another major challenge that needs optimization. Non-convex optimization landscapes, such as barren plateaus that are commonly encountered when training QML models and making parameter tuning very hard are common. More research should therefore be on designing more stable optimization strategies and adaptive training techniques.
- Moreover, system benchmarks of quantum machine learning models on various hardware systems and fields are absent at this time. It will be necessary to have common evaluation criteria and repeatable experimental environments to allow a fair evaluation of new QML algorithms.

Further studies are thus necessary to design noise-resistant quantum algorithms, scalable hybrid quantum-classical learning methods, effective data encoding protocols, and better training algorithms that can run effectively on quantum devices that are available in the near future. The development of quantum hardware, error correction methods, and algorithm optimization will in the near future have a major impact on the way functional quantum machine learning systems are developed.

6. Conclusion

In conclusion, Quantum Machine Learning (QML) is an interdisciplinary area at the interface of quantum computing and machine learning, leveraging the computational benefits of the quantum architecture to boost the analytical power of machine learning algorithms. Based on principles of quantum mechanics, such as superposition and entanglement, QML provides novel learning algorithms able to efficiently solve many high-dimensional optimization problems, for which well-known classical algorithms like gradient descent, coordinate descent or stochastic gradient descent can be very slow, or not even applicable, in practice. Thus, various quantum learning algorithms have been proposed for speeding up tasks like supervised and unsupervised classification, regression, clustering, dimensionality reduction, feature selection and forecasting, ex. by means of Quantum Neural Networks, Quantum Support Vector Machines, and Variational Quantum Circuits. Apart from the development of such new quantum learning algorithms, classical optimization techniques such as gradient-based optimization, Bayesian optimization and evolutionary strategies will play a key role in improving the stability and convergence of quantum learning models. As reflected in the papers presented in this special issue, there are several applications areas, including genomics, disease prediction, environmental science, process optimization, as well as genomics and cheminformatics, where QML is believed to offer significant performance improvements. In spite of these opportunities, there are a number of roadblocks that need to be addressed before the promised performance gains can be realized in practice. In particular, today's quantum processors are still noisy, only have a small number of qubits available, and their current architecture is highly unsuitable for implementing most quantum learning algorithms in an efficient manner. To realize the envisioned performance gains of QML, one needs to improve the quantum processors in several aspects, and complement them with efficient classical pre- and post-processing techniques, such as better data encoding and hybrid quantum-classical learning algorithms. Other applications of quantum computing, time is of

the essence in this regard, and that many of the opportunities that QML can provide for real-world problems in science and engineering will be lost if one does not start to work on them immediately.

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