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Review Article

Quantum Machine Learning Models, Limitations, and Opportunities in the NISQ Era: A Review

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Abstract
Quantum machine learning (QML) has emerged as a promising interdisciplinary field that integrates principles of quantum computing with machine learning techniques to address complex computational challenges. By leveraging quantum phenomena such as superposition and entanglement, QML aims to enhance learning efficiency, improve model performance, and enable the exploration of high-dimensional feature spaces that are intractable for classical methods. This paper presents a comprehensive review of recent developments in QML, covering fundamental concepts, algorithmic taxonomies, data encoding techniques, implementation challenges, and real-world applications. Key approaches, including quantum support vector machines (QSVM), variational quantum circuits (VQC), and quantum neural networks (QNN), are systematically analyzed. Furthermore, critical challenges, including noisy intermediate-scale quantum (NISQ) limitations, barren plateaus, data encoding bottlenecks, and the lack of demonstrated quantum advantage, are discussed in detail. The review also highlights emerging applications in material informatics, energy systems, healthcare, and optimization problems. Finally, future research directions are outlined, emphasizing the need for advancements in quantum hardware, scalable algorithms, hybrid frameworks, and standardized benchmarking. This work aims to provide a structured perspective on the current state of QML and to identify opportunities to deploy it effectively to solve real-world problems.

Keywords: Quantum Machine Learning; Variational Quantum Circuits; Quantum Neural Networks; Quantum Support Vector Machine; NISQ; Quantum Data Encoding.

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1. INTRODUCTION

The rapid advancement of artificial intelligence, particularly in machine learning (ML), has driven significant progress across a wide range of domains, including healthcare, materials informatics, energy systems, and intelligent technologies. However, the increasing complexity of data and the growing demand for computational resources have exposed inherent limitations in classical computing approaches, particularly in terms of scalability and efficiency. In this context, quantum computing has emerged as a promising paradigm that leverages fundamental principles of quantum mechanics, such as superposition and entanglement, to enable potentially exponential computational advantages. The convergence of quantum computing and machine learning has consequently given rise to an interdisciplinary field known as quantum machine learning (QML) [1].

Quantum machine learning aims to develop learning algorithms that can either run on quantum hardware or incorporate quantum principles to enhance classical machine learning techniques. A variety of approaches have been proposed, including quantum-enhanced algorithms such as quantum support vector machines (QSVM), variational quantum circuits (VQC), and quantum neural networks (QNN). These methods exploit the unique properties of quantum systems to accelerate optimization, efficiently explore high-dimensional feature spaces, and potentially improve model generalization [2].

Despite its promising potential, the practical implementation of QML remains constrained by several significant challenges. Current quantum devices operate in the Noisy Intermediate-Scale Quantum (NISQ) era, characterized by limited qubit counts, high error rates, and restricted circuit depths. These limitations often prevent QML algorithms from consistently outperforming their classical counterparts. Furthermore, critical issues such as barren plateaus in optimization landscapes, efficient quantum data encoding (quantum feature mapping), and the integration of hybrid quantum-classical frameworks remain active areas of research [3].

Nevertheless, QML has demonstrated considerable potential across application domains, including material discovery, energy optimization, bioinformatics, and complex signal processing. In the context of

material informatics, QML approaches have been increasingly explored for predicting material properties based on molecular structures, with applications in catalysis, battery technology, and corrosion inhibition. These advancements suggest that QML could significantly accelerate high-throughput screening processes while reducing experimental costs [4].

This review paper provides a comprehensive overview of recent developments in quantum machine learning, covering fundamental concepts, algorithmic frameworks, implementation challenges, and emerging applications. By systematically analyzing the current research landscape, this work seeks to identify key opportunities and future directions for advancing QML technologies.

2. FUNDAMENTAL CONCEPTS

Quantum machine learning (QML) is built on the foundational principles of quantum computing, which differ fundamentally from classical computation. At the core of quantum computing lies the concept of the quantum bit, or qubit, which, unlike a classical bit, can exist in a superposition of multiple states simultaneously. This property enables quantum systems to encode and process vast amounts of information in parallel. Additionally, quantum entanglement enables strong correlations between qubits, allowing operations on one qubit to instantaneously influence others, thereby enhancing computational efficiency for certain classes of problems [5].

Another essential concept in QML is quantum state representation, in which classical data must be encoded into quantum states via a process known as quantum data encoding or quantum feature mapping. Techniques such as amplitude, angle, and basis encoding are commonly used to transform classical datasets into quantum states. The efficiency and effectiveness of this encoding process are critical, as they directly impact the performance and scalability of QML algorithms. Poor encoding strategies can negate potential quantum advantages due to increased circuit complexity or noise sensitivity [6].

Quantum circuits play a central role in QML models, particularly in variational approaches. A quantum circuit consists of a sequence of quantum gates that manipulate qubits to perform computations. In many QML frameworks, parameterized quantum circuits (PQCs), also known as variational quantum circuits (VQCs), are used. These circuits include tunable parameters that are optimized during training, analogous to weights in classical neural networks. The optimization is typically carried out using classical algorithms, resulting in a hybrid quantum-classical learning loop well-suited to current NISQ devices [7].

Measurement is another fundamental aspect of quantum computation, as it is required to extract classical information from quantum systems. After executing a quantum circuit, the quantum state is measured, resulting in a classical outcome. This probabilistic nature of measurement introduces inherent uncertainty, requiring repeated circuit executions (shots) to estimate expectation values accurately. Consequently, the trade-off between accuracy and computational cost becomes an important consideration in QML implementations [8].

Furthermore, the concept of quantum advantage is central to QML's motivation. It refers to the potential of quantum algorithms to outperform classical methods in terms of speed, accuracy, or resource efficiency. While theoretical studies have demonstrated possible exponential speedups for specific problems, achieving practical quantum advantage in real-world machine learning tasks remains an open challenge. This is largely due to hardware limitations and the overhead associated with quantum data encoding and error mitigation [9].

In addition to these core principles, QML also relies on the interplay between classical optimization techniques and quantum computations. Hybrid models, where quantum circuits are embedded within classical machine learning pipelines, have become the dominant approach in current research. This synergy allows researchers to leverage the strengths of both paradigms while mitigating their respective limitations. Overall, understanding these fundamental concepts is crucial for developing efficient and scalable QML models. As quantum hardware continues to evolve, improvements in qubit quality, error correction, and circuit design are expected to further unlock the potential of quantum-enhanced machine learning systems [10].

3. TAXONOMY OF QML ALGORITHMS

Quantum machine learning (QML) algorithms can be broadly categorized based on how quantum computing is integrated into the learning process. In general, QML approaches are divided into three main paradigms: quantum-enhanced classical algorithms, hybrid quantum-classical models, and fully quantum learning models. Each category reflects a different level of quantum involvement and offers distinct advantages and limitations, particularly in the context of current Noisy Intermediate-Scale Quantum (NISQ) devices [11].

The first category, quantum-enhanced classical algorithms, refers to classical machine learning methods that are accelerated or improved using quantum subroutines. A prominent example is the quantum support vector machine (QSVM), which leverages quantum kernels to map classical data into high-dimensional Hilbert spaces that are difficult to simulate classically. By leveraging quantum feature spaces,

QSVM aims to achieve improved classification performance, particularly for complex, nonlinearly separable datasets. Similarly, quantum versions of principal component analysis (QPCA) and clustering algorithms have been proposed to exploit quantum speedups in linear algebra operations [12].

The second and most widely studied category is hybrid quantum-classical models, which are particularly suitable for NISQ-era devices. These models combine parameterized quantum circuits (PQCs) with classical optimization routines, forming a feedback loop in which the quantum circuits generate outputs, and the classical algorithms iteratively update the parameters. Variational quantum circuits (VQCs) are a key example of this approach, where trainable parameters are embedded in quantum gates and optimized using gradient-based or gradient-free methods. Quantum neural networks (QNNs), which generalize classical neural networks into quantum architectures, also fall under this category. These models have been applied to classification, regression, and generative tasks, demonstrating flexibility and adaptability across domains [13].

Another important class within hybrid models is quantum kernel methods, which bridge classical and quantum paradigms. Instead of training quantum circuits directly, these methods use quantum computers to compute kernel matrices that are then fed into classical algorithms such as support vector machines. This approach reduces the burden on quantum hardware while still exploiting quantum advantages in feature mapping. As a result, quantum kernel methods are often considered one of the most practical near-term applications of QML [14].

The third category, fully quantum learning models, comprises algorithms implemented entirely on quantum hardware, without reliance on classical optimization loops. These include quantum Boltzmann machines and quantum generative models, which aim to model probability distributions using quantum states. While theoretically powerful, these approaches remain largely experimental due to the current limitations of quantum devices, particularly in terms of noise and scalability. In addition to these categories, QML algorithms can also be classified by application domain, such as supervised, unsupervised, and reinforcement learning. Supervised QML models, including QSVM and QNN classifiers, are the most mature and widely studied. Unsupervised approaches, such as quantum clustering and quantum autoencoders, are gaining attention for their potential in feature extraction and dimensionality reduction. Meanwhile, quantum reinforcement learning is an emerging area that explores how quantum systems can enhance decision-making processes in dynamic environments [15].

Despite the diversity of QML algorithms, a common challenge across all categories is the effective utilization of quantum resources. Issues such as circuit depth limitations, noise sensitivity, and optimization instability, particularly the barren plateau problem, continue to hinder practical performance. Consequently, ongoing research focuses on developing more efficient circuit architectures, noise-resilient training strategies, and better hybrid frameworks. Overall, the taxonomy of quantum machine learning algorithms highlights the field's evolving landscape, where hybrid approaches currently dominate due to their practicality, while fully quantum models represent long-term aspirations. Understanding these categories provides a structured perspective for evaluating existing methods and identifying promising directions for future research.

4. QUANTUM DATA ENCODING

One of the most critical steps in quantum machine learning (QML) is encoding classical data into quantum states, commonly referred to as quantum data encoding or quantum feature mapping. Since quantum computers inherently operate on quantum states, any classical dataset must first be transformed into a suitable quantum representation before processing can occur. The efficiency, scalability, and expressivity of this encoding process significantly influence the overall performance of QML models, often determining whether a quantum advantage can be realized [16].

Several encoding strategies have been proposed, each with distinct trade-offs between resource requirements and representational power. One of the most widely discussed methods is amplitude encoding, in which classical data are encoded in the amplitudes of a quantum state. This approach is highly memory-efficient, as it can represent (2^n) data points using only (n) qubits. However, preparing such states generally requires complex quantum circuits, which may negate their theoretical advantages, especially on NISQ devices with limited coherence times. Another commonly used approach is angle encoding (also known as rotation encoding), where classical features are mapped to rotation angles of quantum gates, such as (Rx), (Ry), or (Rz). This method is relatively easy to implement and well-suited for current quantum hardware due to its shallow circuit depth. As a result, angle encoding is frequently used in variational quantum circuits (VQCs) and quantum neural networks (QNNs). Despite its practicality, angle encoding may require more qubits or additional circuit layers to effectively capture complex data distributions [17]. Basis encoding represents classical data using computational basis states, mapping binary features directly to qubit states. While conceptually simple and easy to implement, this approach is typically inefficient for representing continuous or high-dimensional data, as it requires a large number of qubits proportional to the dataset size. Consequently, basis encoding is less commonly used in advanced QML

applications, but remains useful for specific discrete problems. In addition to these standard techniques, more sophisticated encoding strategies have been developed to enhance the expressive power of quantum models. For instance, quantum feature maps embed classical data into high-dimensional Hilbert spaces via carefully constructed quantum circuits. These feature maps play a central role in quantum kernel methods, where the similarity between data points is evaluated using quantum inner products. By leveraging the exponential dimensionality of quantum states, quantum feature maps aim to capture complex correlations that are difficult to represent classically [18].

However, the process of quantum data encoding introduces several challenges. One major issue is the data-loading problem, which refers to the difficulty of efficiently transferring large classical datasets to quantum systems. In many cases, the cost of encoding data can outweigh the computational advantages offered by quantum algorithms. Additionally, encoding schemes must be carefully designed to balance circuit depth and noise resilience, as deeper circuits are more susceptible to decoherence and operational errors. Another important consideration is the trade-off between expressivity and trainability. Highly expressive encoding schemes can map data into complex quantum states, but they may also lead to optimization difficulties, including the emergence of barren plateaus where gradients vanish exponentially. This makes training QML models increasingly challenging as system size grows [19].

Recent research has focused on developing adaptive, problem-specific encoding strategies and hybrid approaches that combine classical preprocessing with quantum feature mapping. These efforts aim to reduce encoding overhead while preserving the advantages of quantum-enhanced learning. In particular, domain-informed encoding, such as incorporating molecular descriptors in material informatics, has shown promise in improving model performance and interpretability. In summary, quantum data encoding is a foundational component of QML that directly impacts model efficiency, scalability, and performance. While various encoding techniques offer different benefits, no universal solution currently exists, and the choice of encoding method remains highly problem-dependent. As quantum hardware and algorithm design continue to evolve, more efficient and robust encoding strategies are expected to play a key role in unlocking the full potential of quantum machine learning.

5. CHALLENGES AND LIMITATIONS IN QML

Despite the promising potential of quantum machine learning (QML), its practical realization is still hindered by a range of fundamental and technical challenges. One of the most significant limitations arises from the current state of quantum hardware, which operates in the Noisy Intermediate-Scale Quantum (NISQ) era. These devices are characterized by a limited number of qubits, short coherence times, and high gate error rates. As a result, quantum circuits must remain shallow to maintain reliability, restricting the complexity of QML models and limiting their scalability for real-world applications [20].

Another major challenge lies in optimizing parameterized quantum circuits (PQCs), particularly due to the phenomenon known as the barren plateau. In such cases, the gradient of the cost function becomes exponentially small as the system size increases, making training extremely difficult or even infeasible. This issue is particularly pronounced in deep quantum circuits and can significantly affect the performance of variational quantum algorithms, such as quantum neural networks (QNNs) and variational quantum circuits (VQCs). Addressing this problem requires careful circuit design, initialization strategies, and alternative optimization techniques [21].

The data encoding process also introduces substantial limitations. As discussed previously, efficiently loading classical data into quantum systems remains a non-trivial task. The so-called data loading bottleneck can negate any potential computational advantage offered by quantum algorithms. Furthermore, different encoding strategies present trade-offs between expressivity and resource requirements, making it challenging to identify optimal representations for diverse datasets. Scalability is another critical concern in QML. While theoretical models suggest exponential advantages in certain scenarios, these benefits are often difficult to realize in practice due to hardware constraints and algorithmic overhead. Many QML algorithms require repeated circuit executions (shots) to estimate expectation values, thereby increasing computational cost. Additionally, integrating quantum and classical components into hybrid models introduces latency and communication overhead, further reducing efficiency. Noise and error accumulation present additional obstacles. Quantum systems are highly sensitive to environmental disturbances, which can lead to decoherence and loss of quantum information. Error mitigation techniques have been proposed to alleviate these issues, but they often come with additional computational overhead and are not yet sufficient for large-scale applications. The lack of fully developed quantum error correction further limits the reliability of QML implementations [22].

Another important limitation is the lack of clear and consistent evidence of quantum advantage in practical machine learning tasks. While theoretical studies and small-scale experiments have demonstrated potential benefits, many QML models have yet to outperform well-optimized classical algorithms on real-world datasets. This raises important questions about the conditions under which QML can provide meaningful improvements and highlights the need for more rigorous benchmarking. Moreover,

interpretability and transparency remain underexplored in QML. Unlike classical machine learning models, where interpretability techniques are well developed, understanding the decision-making process of quantum models remains an emerging area. This limitation may hinder the adoption of QML in sensitive applications such as healthcare and finance, where explainability is crucial. Finally, the lack of standardized frameworks, datasets, and evaluation protocols poses a challenge for the systematic development of QML. The field is still in its early stages, with rapid evolution and diverse approaches, making it difficult to compare results across studies. Establishing benchmarks and best practices will be essential for advancing QML research and ensuring reproducibility [23].

In summary, while QML holds significant promise, it faces substantial challenges related to hardware limitations, optimization difficulties, data encoding, scalability, and practical validation. Overcoming these barriers will require coordinated advances in quantum hardware, algorithm design, and hybrid computational frameworks. Addressing these limitations is crucial for transitioning QML from a theoretical concept to a practical tool capable of solving complex real-world problems.

6. APPLICATIONS OF QML

Quantum machine learning (QML) has begun to demonstrate its potential across a wide range of application domains, particularly in areas where classical machine learning faces limitations due to high-dimensional data, complex interactions, or computational constraints. Although still in its early stages, QML is increasingly being explored as a tool to accelerate discovery, improve predictive performance, and enable new forms of data analysis that are difficult to achieve with classical approaches. One of the most promising application areas of QML is in material informatics, where the discovery and optimization of novel materials often require exploration of vast chemical and structural spaces. QML models, such as quantum kernel methods and variational quantum circuits, have been used to predict material properties from molecular descriptors and quantum representations. In particular, QML has shown potential in catalysis research, including the prediction of activity for reactions such as the oxygen evolution reaction (OER), where complex electronic interactions play a critical role. By leveraging quantum feature spaces, QML can capture subtle correlations in molecular structures that classical models may find difficult to learn efficiently [24].

In the field of energy storage, QML is being investigated for applications in battery materials, including lithium-ion and emerging sodium-ion systems. Predicting properties such as ionic conductivity, stability, and electrode performance typically involves highly nonlinear relationships and large datasets. QML approaches can enhance candidate-material screening by enabling more efficient exploration of chemical design spaces. This is particularly relevant for high-throughput computational frameworks, where reducing simulation costs and time is essential for accelerating innovation. Another important application domain is healthcare and bioinformatics. QML has been explored for tasks such as disease classification, drug discovery, and genomic data analysis. Quantum-enhanced models can potentially improve pattern recognition in complex biological datasets, where interactions are often nonlinear and multidimensional. For example, quantum neural networks (QNNs) and quantum support vector machines (QSVMs) have been applied to classify medical images and detect disease-related patterns. Although current results are still preliminary, they suggest that QML could contribute to more accurate and efficient diagnostic systems in the future [25].

In addition, QML has shown promise in financial modeling and optimization problems. Financial datasets are often characterized by high dimensionality, noise, and dynamic behavior, making them well-suited to quantum-enhanced approaches. Applications include portfolio optimization, risk analysis, and fraud detection. Quantum algorithms may offer advantages in solving complex optimization problems and identifying hidden patterns in large-scale financial data. Another emerging area is the application of QML in signal processing and communication systems. Tasks such as pattern recognition, anomaly detection, and time-series forecasting can potentially benefit from the high-dimensional representation capabilities of quantum systems. Quantum-enhanced feature spaces may allow more efficient extraction of relevant information from complex signals, improving the performance of learning models in domains such as wireless communication and sensor networks [26].

Despite these promising developments, most current QML applications remain at the proof-of-concept stage. The limitations of quantum hardware, including noise and scalability constraints, continue to restrict large-scale deployment. As a result, many studies rely on simulations or hybrid quantum-classical frameworks rather than fully quantum implementations. Nevertheless, the integration of QML into real-world applications is expected to grow as quantum technologies mature. In particular, domains that inherently involve quantum phenomena, such as chemistry, materials science, and physics, are likely to benefit the most from QML approaches. By aligning computational models more closely with the underlying physical processes, QML has the potential to unlock new levels of accuracy and efficiency [27]. In conclusion, while still in its infancy, quantum machine learning spans diverse fields, with particular potential in material informatics, energy systems, healthcare, finance, and signal processing.

Continued advancements in both quantum hardware and algorithm design will be essential for translating these early successes into practical, large-scale solutions.

7. FUTURE DIRECTIONS AND RESEARCH OPPORTUNITIES

As quantum machine learning (QML) continues to evolve, several promising research directions are emerging that could significantly enhance its practical impact and accelerate its transition from theoretical exploration to real-world applications. One of the most critical areas for future development is advancing quantum hardware. Improvements in qubit quality, coherence times, and error-correction mechanisms are essential to enabling deeper, more reliable quantum circuits. The transition beyond the Noisy Intermediate-Scale Quantum (NISQ) era toward fault-tolerant quantum computing is expected to unlock the full potential of QML algorithms. Another important direction lies in the design of more efficient and scalable quantum algorithms. Current QML models often struggle with optimization challenges, including the presence of barren plateaus and sensitivity to noise. Future research should focus on developing novel circuit architectures, initialization strategies, and training techniques that improve convergence and stability. In particular, adaptive and problem-specific variational circuits may offer a pathway toward more robust learning models [28].

Quantum data encoding remains a fundamental bottleneck that requires further innovation. Developing encoding techniques that are both resource-efficient and expressive is crucial for achieving meaningful quantum advantage. Hybrid strategies that combine classical preprocessing with quantum feature mapping are expected to play a key role in addressing this challenge. Additionally, leveraging domain knowledge, such as physicochemical descriptors in material informatics, can lead to more effective and interpretable encoding schemes. The integration of QML with classical machine learning frameworks is another promising avenue. Hybrid quantum-classical systems are likely to remain the dominant paradigm in the near term, and improving the interoperability between quantum circuits and classical pipelines will be essential. This includes the development of optimized interfaces, efficient gradient estimation methods, and scalable training workflows. Advances in this area could enable seamless incorporation of quantum components into existing machine learning ecosystems [29].

Benchmarking and standardization also represent critical research needs. The lack of widely accepted benchmarks, datasets, and evaluation protocols makes it difficult to assess the true performance of QML models compared to classical approaches. Establishing standardized evaluation frameworks will not only improve reproducibility but also provide clearer insights into where quantum advantages can be achieved. Comparative studies between classical and quantum models on real-world datasets will be particularly important in this regard. Another emerging research direction is the exploration of application-specific QML models. Rather than developing general-purpose algorithms, future work may focus on tailoring QML approaches to specific domains such as material discovery, quantum chemistry, and energy systems. In these areas, the alignment between quantum computational models and the underlying physical processes may provide a natural advantage over classical methods. For instance, integrating QML with high-throughput computational screening in material informatics could significantly accelerate the discovery of novel catalysts and energy materials. Interpretability and explainability are also expected to become increasingly important as QML matures. Developing methods to understand and visualize the behavior of quantum models will be crucial for building trust and facilitating adoption in sensitive domains such as healthcare and finance. This includes creating tools for analyzing quantum circuits, feature importance, and decision boundaries in quantum-enhanced models [30].

Finally, interdisciplinary collaboration will play a vital role in advancing QML research. The field inherently sits at the intersection of quantum physics, computer science, mathematics, and domain-specific applications. Collaborative efforts that bring together expertise from these areas are essential for overcoming current limitations and driving innovation. In summary, the future of quantum machine learning is both challenging and promising. Key research opportunities lie in improving quantum hardware, developing scalable algorithms, optimizing data encoding, enhancing hybrid frameworks, and establishing standardized benchmarks. As these challenges are progressively addressed, QML is expected to evolve into a powerful tool capable of solving complex problems that are currently intractable for classical machine learning methods.

8. CONCLUSION

Quantum machine learning (QML) represents a rapidly evolving research frontier that seeks to combine the computational power of quantum mechanics with the adaptability of machine learning. This review has provided a comprehensive overview of QML, covering its fundamental principles, algorithmic taxonomy, data encoding strategies, implementation challenges, and emerging applications across multiple domains. Through this discussion, it is evident that QML offers a novel paradigm with the potential to address complex problems that are difficult or inefficient to solve using classical approaches.

Despite its theoretical advantages, the current state of QML remains largely constrained by hardware limitations of the *Noisy Intermediate-Scale Quantum* (NISQ) era. Issues such as limited qubit availability, noise sensitivity, barren plateaus in optimization, and inefficient data encoding continue to pose significant challenges. These limitations often prevent QML models from consistently outperforming classical machine learning methods in practical settings. As a result, most successful implementations to date rely on hybrid quantum-classical frameworks that balance feasibility and performance. Nevertheless, the potential applications of QML are extensive and particularly promising in domains that inherently involve quantum phenomena, such as material informatics, quantum chemistry, and energy systems. In these areas, QML has demonstrated early success in tasks such as property prediction, catalyst discovery, and high-throughput screening. Additionally, applications in healthcare, finance, and signal processing suggest that QML could eventually play a transformative role across a broad range of industries. Looking forward, the realization of practical QML will depend on coordinated advancements in both quantum hardware and algorithm design. Improvements in qubit quality, error correction, and scalable architectures will be essential for enabling more complex and reliable quantum computations. At the same time, the development of efficient encoding methods, robust optimization strategies, and standardized benchmarking frameworks will be critical for advancing QML research and validating its advantages over classical techniques. In conclusion, while quantum machine learning is still in its early stages, it holds significant promise as a next-generation computational paradigm. Continued interdisciplinary research and technological progress are expected to gradually overcome current limitations, paving the way for QML to become a powerful tool in solving real-world problems and advancing scientific discovery.

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