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Artificial intelligence (AI) for quantum and quantum for AI

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Abstract
The technological fields of AI and quantum technology have evolved in parallel, and have demonstrated considerable potential to complement each other. Amalgamation of them refers to the use of AI techniques to develop algorithms for quantum computing (QC) and quantum physics, as well as the use of QC to enhance AI applications. QC has the potential to revolutionize various fields. Controlling quantum systems is notoriously difficult, which is one of the major obstacles standing in the way of widespread use of QC. AI has opened up new avenues for automated control of quantum systems. In particular, the application of AI can provide invaluable insight into the complex and multifaceted domain of quantum physics to accelerate the discovery of quantum physics laws, and can potentially alleviate challenges that have been historically associated with QC and quantum communication. On the other hand, QC can also be used to enhance AI applications. For instance, QC can be used to haste the training of neural networks, which are used in machine learning. Concurrently, a series of advancements in quantum technology can serve to drive innovation in the realm of machine learning by enabling the development of novel algorithms, frameworks, and hardware. This article presents a comprehensive overview on the reciprocal relationship between AI and quantum technology, emphasizing the utility of AI in the field of quantum technology, and the potential of quantum technology to catalyze the evolution of AI.

Keywords AI, machine learning · Frameworks · Quantum computing · Quantum technology

1 Introduction

The emergence of AI and quantum technology has been characterized by a tumultuous developmental trajectory over the last several decades, ultimately culminating in the advent of technological advancements that have the potential to fundamentally transform the fabric of human innovation, production, and daily life, as illustrated in Figs. 1 and 2.

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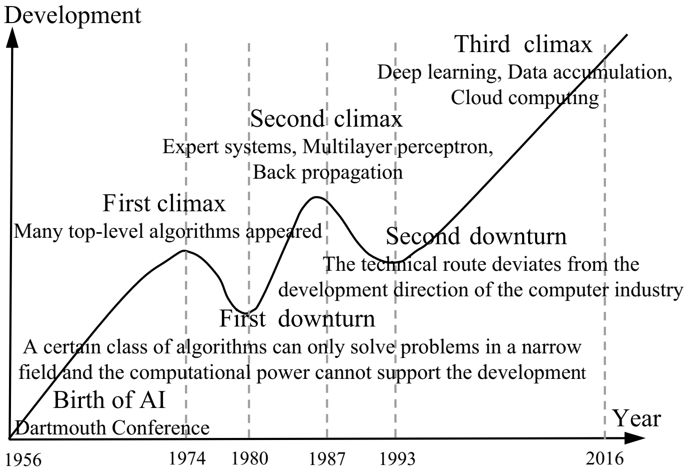
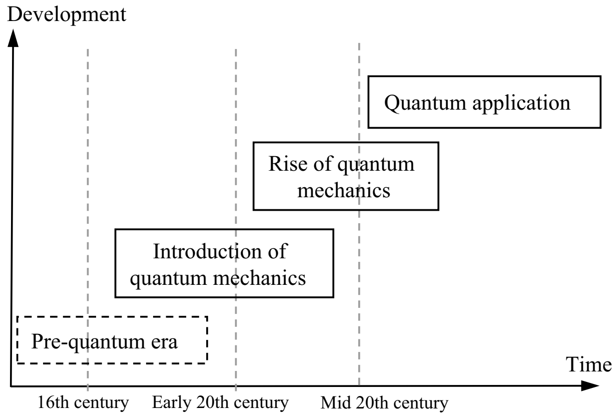


Fig. 1 AI development history so far

Fig. 2 Quantum technology development history



Nevertheless, the reliability of Moore's law has diminished in recent years, and the capacity of classical computers is now increasingly strained, with traditional hardware stacking methods being insufficient to accommodate the soaring demand for computational power required by complex AI models. As a result, the future development of AI may potentially enter a winter period. Moreover, the ultimate potential of quantum technology remains largely uncharted, with many barriers currently obstructing its widespread adoption, some of which may necessitate the aid of AI to overcome.

Given these circumstances, a critical research direction involves strategic integration of these two nascent technology fields in order to fully leverage their potential synergies and promote mutual growth, as illustrated in Fig. 3. This highlights the significant potential for the ongoing interaction between quantum technology and AI to emerge as a defining trend in the field.

Significant research has been conducted in cross-disciplinary collaboration and mutual enhancement between AI and quantum technology. On the one hand, AI has demonstrated considerable utility in addressing complex quantum problems and

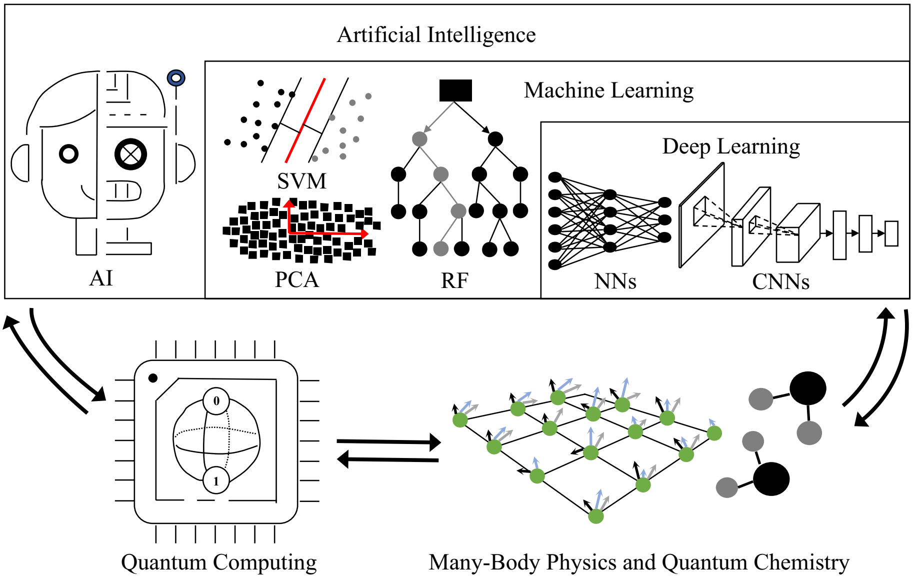


Fig. 3 Interaction between AI and quantum technology

supporting quantum physicists in the analysis of challenging quantum physics data, such as phase transitions identification, quantum state classification, quantum entanglement processing, and ground state energy estimation. QC technology has contributed to the advancement of AI by providing theoretically accelerated versions of classical ML algorithms and facilitating the emergence of quantum neural networks (QNNs). Notably, recent research has demonstrated that the simulation capabilities of single-bit QNNs are comparable to the general approximation theory of classical neural networks (Yu, et al. 2022). QNNs can be expressed in terms of Fourier series with L-term truncation.

1.1 Objectives of the study

- The study provides a general overview of the potential synergies and mutual growth opportunities between the fields of AI and quantum technology.
- The main results of the article focus on the significant research that has been conducted in cross-disciplinary collaboration and mutual enhancement between AI and quantum technology.
- The article highlights the utility of AI in addressing complex quantum problems and supporting quantum physicists in the analysis of challenging quantum physics data, while quantum technology has contributed to the advancement of AI by providing theoretically accelerated versions of classical ML algorithms and facilitating the emergence of quantum neural networks (QNNs).

- The article also notes recent research demonstrating the simulation capabilities of single-bit QNNs comparable to the general approximation theory of classical neural networks.

1.2 The major highlights of the research study on "AI for Quantum and Quantum for AI" are:

a) The potential for AI and quantum technology to work together synergistically and revolutionize the fields of ML and pattern recognition.
b) The current limitations of classical computing in accommodating the computational demand of complex AI models, leading to the need for quantum computing.
c) The potential of quantum computing to address complex optimization problems and improve data analysis, leading to potential benefits in AI and other fields.
d) The emergence of quantum machine learning and quantum neural networks as promising areas of research.
e) The ethical implications of AI and quantum computing, including issues around data privacy and security, and the need for responsible development and deployment of these technologies.
f) The importance of cross-disciplinary collaboration and mutual enhancement between AI and quantum technology to fully leverage their potential synergies and promote mutual growth.

1.3 Potential role of AI in developing quantum algorithms

The AI techniques that have been used for developing the quantum algorithms are mentioned below.

- *Variational quantum algorithms (VQAs)*: VQAs are a class of algorithms that use AI techniques to optimize quantum circuits. These algorithms can learn to adjust the parameters of a quantum circuit in real-time, allowing for the development of more efficient quantum algorithms.
- *Quantum generative adversarial networks (QGANs)* QGANs are a type of generative model that use quantum circuits to generate data. Researchers have used QGANs to develop quantum algorithms that can generate samples from complex quantum systems, such as molecules.

These AI techniques have shown promising results in developing quantum algorithms, but there is still much research to be done in this area. It is likely that future breakthroughs in quantum computing will rely on a combination of AI and traditional algorithm development techniques.

1.4 The paper organization

The paper is structured into six sections. The article begins with the introduction section, followed by the highlights on AI and quantum computing. The third section elaborates the role of AI for quantum computing. The fourth section elaborates the quantum for AI. Then the fifth section discusses the ethics for implications of AI and quantum computing in real world scenario and the last section concludes the research study.

2 AI and Quantum

The integration of quantum technology and AI has appeared as a critical zone of investigation with vast potential. The application of AI to quantum technology offers an efficient means to address complex quantum problems, particularly as Moore's Law approaches its physical limits. Going forward, quantum technology may serve to accelerate the advancement of AI at the application end of the industry. The interplay of quantum technology and AI is poised to become an exciting driver of economic and social development, representing a significant opportunity for future growth and innovation.

2.1 AI uncover mystery of quantum physics

The mainstream approaches in AI currently comprise supervised learning (SL0, reinforcement learning (RL) and unsupervised learning (UL) (Carleo et al. 2019). SL involves the deduction of prediction functions from marked training data, where each instance includes both input and expected output, allowing for the estimation of tags based on the data provided. Unsupervised learning, on the other hand, involves the inference of conclusions from unmarked training data. Cluster analysis, a typical unsupervised learning method, is useful for discovering hidden patterns or grouping data during exploratory data analysis, with the aim of finding the hidden structure of the data. RL is focused on enabling software agents to take activities in an environment, with the aim of boosting cumulative returns. Specifically, it aims to learn how to select a sequence of actions that will result in long-term benefits given a particular set of data.

Moreover, the architecture and algorithms used in supervised learning, unsupervised learning, and RL are versatile and extendable, making them suitable for use in quantum physics and other branches of physics. Specifically, these approaches can be applied to perform numerous functions in sturdily allied systems, quantum computing and matter, and physics statics (Dawid, et al. 2022).

While AI and quantum physics may seem disparate, they share many similarities in terms of their ability to extract information and rules. AI is, in essence, an optimization problem that aims to find the optimal solution by optimizing parameters in a multi-parameter space. One potential application of AI to quantum physics is parameter optimization control, which can help to train data more cost-effectively. This is especially useful in the field of physics research, where the control of experimental parameters typically involves adjusting many parameters in the laboratory, resulting in high energy consumption. The mathematical description of experimental parameters involves optimizing quantifiable control parameters to help the experimental system achieve control objectives. However, the mapping function between experimental control parameters and the experimental target is highly complex, making it difficult to find the extreme point of the mapping function without the help of AI. Although quantum physics data points are often lacking, it is still possible to use AI to fit this complex function and find its extreme point, which is useful for discovering the underlying laws of quantum physics.

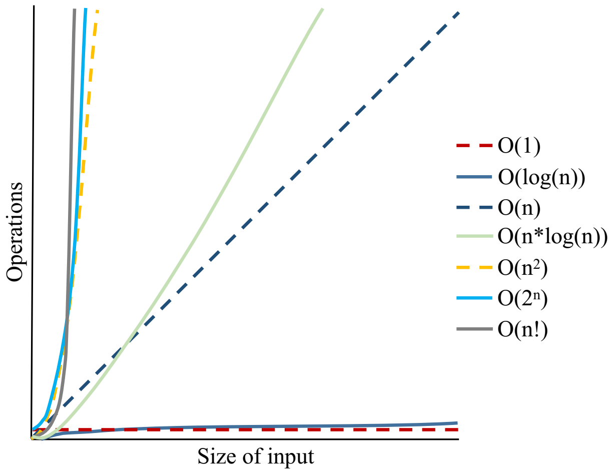


Fig. 4 Time complexity

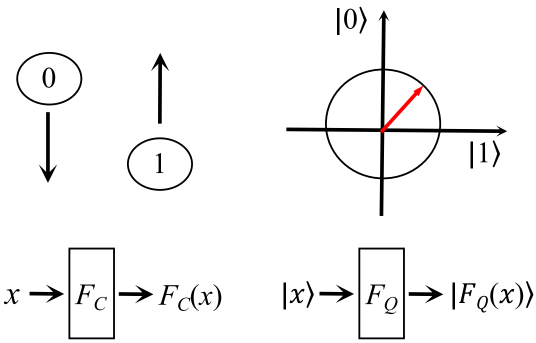


Fig. 5 Traditional bit and qubit

2.2 Developing AI by quantum computing

The advancement of QC has enabled the development of more powerful AI algorithms that can significantly reduce algorithm runtime and improve algorithm performance (Vivas, et al. 2022). This is particularly useful for tasks that have high computational complexity, particularly those involving exponential complexity problems, such as n2 or 2n, as demonstrated in Fig. 4.

In order to tackle the challenges in AI, improved models and algorithms alone are insufficient, as faster computational methods are also crucial. Quantum computing presents a promising avenue for achieving this goal. By combining the characteristics of quantum superposition, quantum tunneling, and quantum entanglement, quantum computing provides an alternative method for data processing that surpasses classical computing.

Classical computing processes data using a binary system of 0 s and 1 s. In contrast, a single qubit in quantum computing can hold two values, 0 or 1, which are represented by the notations $|0\rangle$ and $|1\rangle$, respectively, as illustrated in Fig. 5. Therefore, a qubit can be denoted by a linear superposition of these two states, which is given by.

$$q = a|0 + b|1 , \tag{1}$$

$$|0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{2}$$

$$|1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{3}$$

$$|a|^2 + |b|^2 = 1, \tag{4}$$

where a and b are the amplitudes and are a linear combination of $\left|0\right\rangle$ and $\left|1\right\rangle$.

In a three-dimensional space, a sphere can be obtained by scanning all directions while rotating around the x and z axes. This sphere can be used to visualize qubits, as depicted in Fig. 6. Specifically, $\left|0\right\rangle$ and $\left|1\right\rangle$ are located at the north and south poles of the sphere, respectively, while other positions on the sphere can be obtained by multiplying the cosine and sine functions of the corresponding angles.

Classical computing is limited in its ability to represent data, as the information stored in N bits only represents one data, despite there being 2^N possible outcomes. In contrast, quantum computing enables the superposition of 0 and 1, allowing multiple qubits to act coherently to represent the data of 2^N. For instance, in a hypothetical experiment involving a cat and a small amount of radioactive material enclosed in a box, classical physics dictates that the cat will either live or die. However, in the quantum world, if the box is not opened, the cat inside will exist in a superposition of both alive and dead states.

Quantum entanglement is a phenomenon that arises when the properties of particles become integrated into the overall properties of the system after interacting with each other, making it impossible to describe the individual properties of each particle. This phenomenon is made possible by superposition. See Fig. 7 for a visual representation of how the detection of one entangled qubit may be used to infer the configuration of the other.

Superposition and entanglement, when combined, enable exponential growth of computer power in quantum computing. Specifically, adding each new qubit to a quantum system doubles the number of states that can be analyzed, which is in stark contrast to the limitations of classical computing. This provides a significant speed increase for AI applications.

Quantum interference is a critical aspect of quantum computation. The amplitudes of two wavelet functions can be enhanced when their phases are identical. Conversely, the amplitudes will be weakened when the phases of two wavelet functions are opposite. Figure 8 provides a visual representation of this phenomenon.

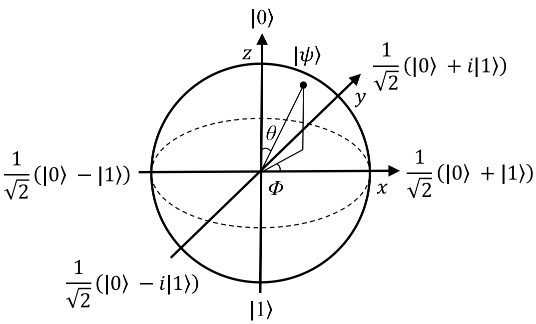


Fig. 6 Bloch sphere

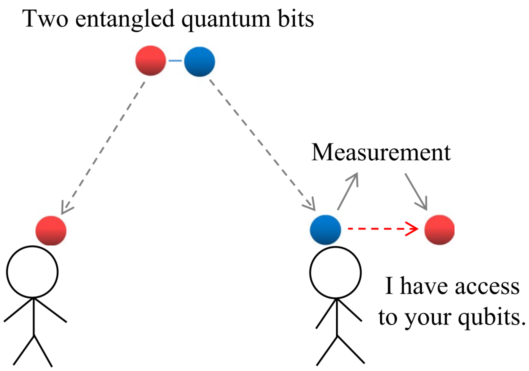


Fig. 7 Quantum teleportation

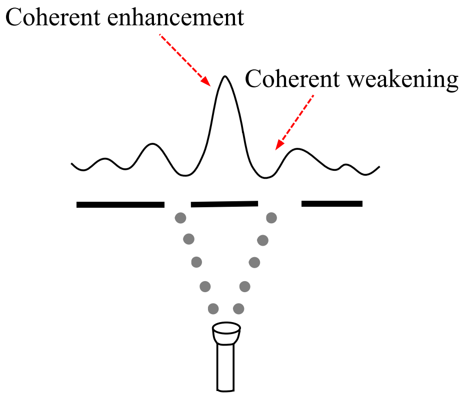


Fig. 8 Interference phenomenon

Thanks to them, QNN, a novel model that integrates the features of quantum mechanics theory with neural networks, represents a significant breakthrough in the field. Despite the construction of the quron, there are still several obstacles that need to be overcome. One such challenge is the unification of the nonlinear dissipation dynamics of neural computing with the linear and single dynamic process of quantum computing, which presents a formidable challenge for implementing QNN.

Research into ML algorithms founded on the framework of quantum computing is expected to play a crucial part in progressing the realization of ML on quantum computers and promoting the development of quantum ML.

Quantum machine learning (QML) is a rapidly growing field that combines the principles of quantum mechanics with machine learning. It aims to develop algorithms and techniques that can leverage the inherent advantages of quantum computers to solve complex problems in machine learning and pattern recognition. These advantages include the ability to perform parallel computations, the ability to represent and manipulate large amounts of data simultaneously, and the ability to use quantum entanglement to perform computations that would be impossible on classical computers.

Quantum neural networks (QNNs) are a specific type of qml model that uses quantum circuits to perform computations. QNNs can be used for classification, regression, and clustering. They are particularly useful for problems that involve large amounts of data, as they can process many inputs simultaneously.

The potential impact of QML and QNNs is significant. They have the potential to revolutionize fields such as drug discovery, financial modeling, and cryptography by enabling faster and more accurate analysis of large datasets. They also have the potential to solve problems that are currently intractable for classical computers.

Despite the promising potential of QML and QNNs, the field is still in its early stages and faces several challenges. These include the need for more powerful and reliable quantum hardware, the development of efficient quantum algorithms, and the need for more research to understand the theoretical foundations of QML and QNNs.

3 AI for quantum

The effectiveness of AI in solving numerous challenges related to quantum physics has been well documented, and its range of applications has continued to expand. These include quantum state representation, quantum phase classification, quantum control, quantum communication, and error correction.

AI and quantum computing have the potential to impact various fields beyond machine learning and optimization. Some possible applications of AI and quantum computing in the current era include:

- *Chemistry and drug discovery* Quantum computing can simulate molecular structures and properties to accelerate drug discovery and material design. AI can help analyze large amounts of chemical and biological data to aid in the discovery process.
- *Finance and economics* Quantum computing can optimize portfolio management, risk assessment, and financial modeling. AI can assist in predicting stock prices and market trends.
- *Cybersecurity* Quantum computing can break traditional encryption methods, but it can also enhance security by generating unbreakable cryptographic keys. AI can improve threat detection and response through advanced analytics and automation.
- *Transportation and logistics* Quantum computing can optimize routing and scheduling for vehicles and transportation networks. AI can enhance predictive maintenance and real-time traffic management.
- *Climate modeling* Quantum computing can simulate complex climate models and optimize energy systems. AI can help analyze satellite and sensor data for weather forecasting and disaster response.

The potential applications of AI and quantum computing are vast and far-reaching, with the potential to impact nearly every industry and field.

3.1 AI for quantum states

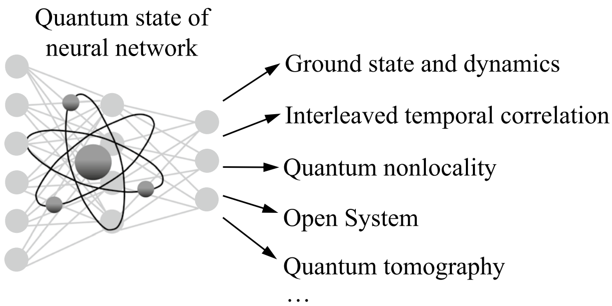
For several decades, quantum many-body physics has been a fundamental and challenging subject in condensed matter physics. The intricate nature of these systems has been a problem for physicists since the 1930s, with the difficulty of solving the equations involved being one of the main issues. The computation of Hilbert space dimensions increases exponentially as the wave function is solved, resulting in the exponential wall phenomenon. Tensor network states and matrix product states were introduced as ways to address this challenge. These methods accurately represent the ground state and other states of a multi-form structure through the state reduced by small tensors, resulting in a significant decrease in numerical complexity.

The emergence of artificial intelligence has spurred the development of the neural network quantum state (NNQS) approach to solve complex problems, which has gained significant attention. This method uses a neural network and adjusts network parameters to approximate the target wave function, such as the ground state of a multi-body system. In the context of solving quantum many-body phenomena, it is a potent variational computing approach. Compared to tensor network states, The top limit of NNQS's expressiveness is considerably greater for the same number of parameters, and it may effectively depict quantum states with high entanglement entropy.

The use of restricted Boltzmann machines (RBMs) has become increasingly common in NNQS studies. Recursive backpropagation (RBM) is a multiple network with an exposed layer and an underlying concealed layer. Visible layer neurons can make connections to hidden layer neurons, but not to other neurons in the same layer. RBM can estimate any smooth function to arbitrarily high accuracy when the hidden layer has a sufficient number of neurons. RBM is capable of representing every possible quantum state. For a given number of neurons in the visible layer and in hidden layer neurons grow at a polynomial rate, indicating that the number of attributes required expressing the quantum condition in terms of RBM is not growing exponentially. Approximating the ground state representation of archetypal systems in condensed matter physics using the RBM wave function has shown to be a fruitful effort (Carleo and Troyer 2017; Nomura 2021). Carleo and Troyer (2017) has compared and verified the RBM method with traditional density matrix renormalization group methods in Heisenberg models, fully demonstrating the advantages of the RBM neural networks. In addition to solving the ground state and dynamic evolution of quantum systems, it can also be applied to quantum state tomography (QST) (Meng et al. 2022) and solving the steady state problems in the complex systems (Yoshioka and Hamazaki 2019). Quantum state characterization, or QST, is the method through which a thing's quantum state is defined in detail.

The RBM, while useful for approximating certain quantum states, is known to have limited representational capability due to its simple structure. For example, some quantum states, such as two-dimensional cluster states obtained by special unitary transformations, cannot be expressed by RBMs. To address this limitation, a hidden layer can be added to the original RBM to obtain a deep Boltzmann machine (DBM). Compared to RBMs, DBMs have exponential advantages in expression ability, as shown in various studies (Nomura et al. 2021).

Fig. 9 Application of quantum states



In addition to RBMs and DBMs, other neural networks can also be used to represent quantum states, with different networks being selected based on specific applications. These applications include ground state and dynamics, interleaved temporal correlation, quantum nonlocality, open systems, and quantum tomography, as shown in Fig. 9.

3.2 AI for quantum phases of matter

The classification capabilities of AI are widely known in the macroscopic world, and are known to surpass human performance in certain contexts. These capabilities are also being applied to quantum many-body systems, particularly in the identification of quantum phases. The probability distribution of quantum states follows a wave-like pattern, in which probability is determined by the amplitude of the wave. The phase of the wave also carries information, as illustrated in Fig. 10. The role of phase in quantum mechanics is remarkable.

In the context of a time-dependent Hamiltonian, the potential field evolves according to a periodic function of time, generating a wave function that is incapable of returning to its initial state after a complete period of evolution. This results in a phase that is related to time, and leads to observable physical effects. The significance of phase extends beyond quantum mechanics, as it also plays a critical role in other areas of physics.

Currently, supervised learning is the most commonly employed classification algorithm for phase of matter identification (Hsu et al. 2018; Ho and Wang 2021; Zhao et al. 2022) . Such algorithms enable the clear detection of new phases, the localization of phase boundaries, and accurate classification. However, for complex multi-body systems with limited theoretical knowledge of simulation models, identifying new physics from a large amount of measured data can be grueling (Lidiak and Gong 2020). To address this issue, UL methods have been developed to discover new phases of matter without any prior theoretical knowledge (Rahaman et al. 2023; Kottmann et al. 2020; Teng et al. 2022). While these methods have proven successful in characterizing phases that exhibit symmetry breaking, identifying topologically similar phases without local sequence parameters remains challenging without supervision. A hybrid approach that combines unsupervised and supervised learning techniques has also emerged as a promising strategy (Miles et al. 2023).

3.3 AI for quantum control

The advancement of quantum control has the potential to enhance human comprehension of the microcosm and regulate the behavior of quantum systems. In contrast to the study of macro-control concerns, quantum control focuses on regulating the behavior of micro-quantum mechanical systems. The objective is to design and implement control through

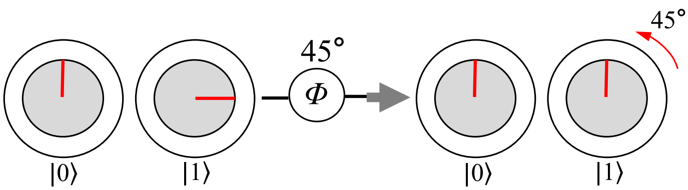


Fig. 10 Phase operation

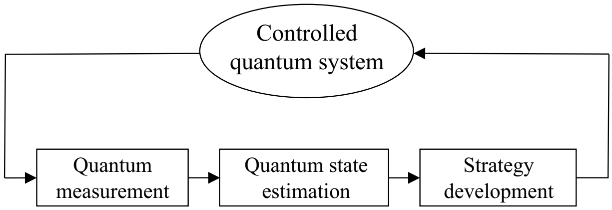


Fig. 11 Architecture of quantum control based on measurement feedback

custom external fields so that the dynamics of quantum systems can evolve in a specific manner.

One noteworthy class of traditional quantum control methods involves measurement feedback techniques (Kaur et al. 2022a), which is presented in Fig. 11. The controlled quantum system requires measurement, and state estimation is carried out using the completeness of the observed quantities. This refers to the computation of the overall state of the system by combining the probability of the quantum state's projection on different mechanical quantities. Hence, the original matrix is reconstructed using the density matrix's projection in various directions. The execution strategy is then fed back to the controlled system based on the assessed system status.

Despite the benefits of measurement in providing system information, quantum mechanics measurements are distinct from classical measurements. The quantum system is prone to collapsing and introducing uncertainty, making it a random system. Additionally, there are other issues during the experiment, such as calibration errors, feedback delays, and inefficient measurement. Quantum control techniques based on measurement feedback still face significant obstacles.

RL has demonstrated remarkable success in classical control applications, and its potential also extends to quantum control. The quantum control framework based on RL is illustrated in Fig. 12.

At each time step, the quantum control agent receives information about the existing enunciate of the quantum circuit and uses this information to determine the appropriate execution strategy. This involves selecting the desired logic gate to be applied from a set of possible gates that could be added to the quantum circuit. The quantum control agent then receives feedback in the form of rewards from the controlled quantum system. Several quantum control methods based on RL have been extensively studied (An et al.

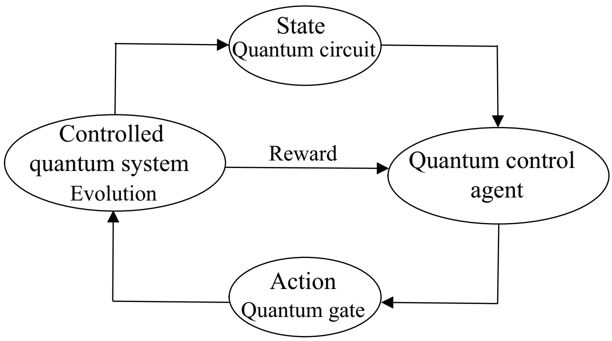


Fig. 12 Quantum control framework based on RL

2021; Wang et al. 2020; Borah et al. 2021). These techniques either provide the quantum regulatory agent with foreknowledge of the quantum express or place significant weight on fidelity as a metric of optimization. It is true that simplifying assumptions may make quantum control issues more manageable for agents, but these assumptions often place significant constraints on the problems' experimental viability (Sivak et al. 2022).

3.4 AI for quantum communication and error correction

Quantum communication (Qc), a nascent communication paradigm that employs quantum superposition states and entanglement effects to transmit information, offers an infallible security guarantee that is impervious to eavesdropping and computational cracking. Capitalizing on the foundational tenets of quantum mechanics, such as the principles of uncertainty, measurement collapse and non-cloning, Qc is poised to catalyze a new era of technological innovation and transform the communication industry. One of the prominent methods of Qc is quantum key distribution (QKD), which securely shares a QK between remote locations through the transmission of quantum states, and encrypts information one bit at a time using the key. The integration of AI can enhance the efficiency and security of QKD. Recent advances in the real-time feedback control of QKD (Liu et al. 2019), parameter optimization and strength selection of QKD systems (Wang and Lo 2019), noise mitigation (Kaur and Kadam 2017), QKD protocol design (Liu et al. 2022; Okey et al. 2022; Kaur et al. 2022b), attack resistance, and resource allocation (Xu et al. 2022) have paved the way for intelligent QKD research. Additionally, AI has the potential to facilitate long-distance quantum communication and optimize quantum receiver strategies (Wallnöfer et al. 2020; Le et al. 2022).

In the realm of communication and computation, errors are an unavoidable phenomenon. Quantum error correction (QEC) is crucial in the context of quantum communication and quantum computing for maintaining the reliability of sensitive quantum systems. The interaction between a quantum system and its surroundings might result in the loss or alteration of system information. As the unit size and number of qubits rise, the system becomes more complex, maintaining strict isolation becomes increasingly challenging. The occurrence of incoherence inevitably leads to errors, which can be classified into two types: bit flip and phase flip. Bit flip pertains to the incorrect change or flip of the calculation state of a quantum bit, causing the state to change from $|1\rangle$ to $|0\rangle$ or vice versa. On the other hand, phase flip involves an incorrect change in the phase of the qubit. Various algorithms have been devised to mitigate the frequency of quantum errors (Hsu et al. 2018). Fault tolerance of quantum systems is also heavily influenced by their error correction capabilities. Surface code, which is the most classical quantum error correction code, can be realized by arranging bits on a surface as depicted in Fig. 13.

However, it needs to satisfy the requirements of the renowned Shor algorithm (Melvin 2022), which may be severely restricted by the no. of qubits and hardware, making it challenging to support large-scale quantum computing and complex quantum systems. Similar issues arise in most traditional quantum error correction schemes.

Quantum error correction is a crucial technique for protecting sensitive quantum systems from environmental interactions. While there exist many algorithms that can suppress the frequency of quantum errors, the error correction capability after the occurrence of an error is a crucial aspect for ensuring the fault tolerance of quantum systems. Traditional quantum error correction schemes have limitations that prevent

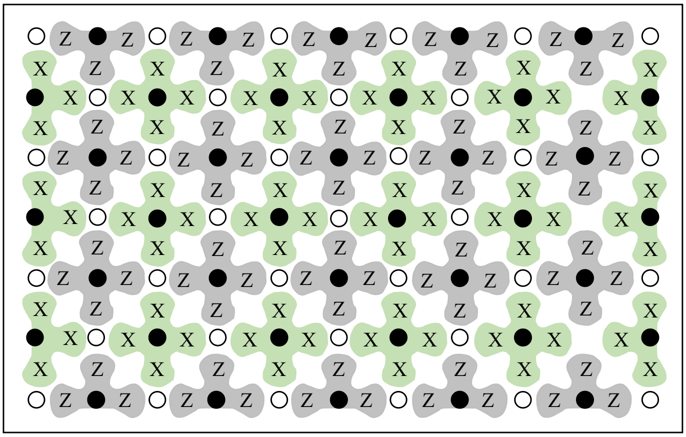


Fig. 13 Surface code

them from supporting large-scale quantum computing and complex quantum systems. In this regard, recent research (Kim et al. 2022a; Stein, et al. 2022; Overwater et al. 2022; Wang et al. 2022) has explored the use of AI for quantum error correction, with a particular focus on multidimensional Bose quantum error correction using neural network decoders. Unlike traditional error correction methods that use bit coding, Bose coding uses light as a carrier, with infinite energy levels in the harmonic oscillator potential. It has been shown that Bose quantum error correction is an effective infinite-dimensional quantum error—correcting approach. Recent research (Wang et al. 2022) has combined the minimal weight perfect matching technique with the curved boson model decoding to dramatically increase the performance of the NN decoder and alleviate the exorbitant hardware requirements. The multi-dimensional combined error correction code method has shown a 15% increase in the decoding threshold compared to the surface code.

4 Quantum for AI

Neural networks, a popular ML algorithm, are increasingly used in complex computing applications. However, their expanding structure and complexity have resulted in bottlenecks in computing speed and performance. To address these issues, Subhash and Ron Chrisley introduced the concept of quantum neural computing in 1995, which exploits the properties of quantum mechanics to enhance cognitive function. Specifically, with the development of technology, QNN is designed to operate on quantum circuits utilizing state superposition, entanglement, interference, and quantum logic gates as basic computing units. QNN takes advantage of neural networks to solve the complex problems.

4.1 QNN

QNN is a novel model that merges the features of quantum mechanics with those of neural networks. Specifically, it constitutes a parameterized quantum circuit where the parameters of the quantum gate are adjustable. This enables the quantum computer to evolve into the desired state, similar to the training process of a classical NN. The main disparity between

QNN and classical neural network lies in the calculation of quantum bits, which is based on state superposition, entanglement, interference, and other properties. Unlike the classical neural network where deepening the network structure and augmenting the parameters may enhance the model's expressiveness to a certain extent, the same operations might not significantly improve the expressiveness of the quantum circuit. In some cases, these parameters may even be deemed superfluous (Sim et al. 2019).

The representation of a multi-bit case requires a higher-dimensional Bloch sphere, as the lower-dimensional version cannot capture the full complexity of the quantum system. Importantly, a quantum circuit does not relate to a physical circuit in quantum computer hardware, but rather to a quantum algorithm that is expressed in a visual format. Similar to how a music score captures the changes in music over time, lines are used to represent the quantum bit state as it evolves over time, as demonstrated in Fig. 14.

To evaluate the efficacy and status of quantum circuits, expressibility, entanglement capacity, and circuit cost are commonly used measures. Expressibility indicates the circuit's ability to generate pure states that represent the Hilbert space, while entanglement capacity measures the degree of entanglement in the system. Circuit cost can be quantified by the number of circuit layers and bit gates employed (Luca 2022).

QNN introduces the concept of quantum state superposition into the traditional feed-forward neural network, where multiple sigmoid functions are used to superimpose the hidden layer excitation function of the NN. Unlike a sigmoid function, which can only represent two orders of magnitude and states, there exist different quantum intervals between adjacent sigmoid functions of linear superposition. By using a hidden neural unit, a greater number of orders of magnitude and states can be represented, enabling the quantification of the uncertainty of the input data of the training sample and mapping different data to different orders of magnitude through the training of quantum interval. A multi-layer excitation feature is used to enhance the fuzziness of the system, hence enhancing the precision and confidence of network pattern identification. The quantum neuron model replaces the weight vector of the perceptron with a wave function, which is the quantum coherent superposition of all possible classical weight vectors. As the superimposed weight vector interacts with the environment, such as when stimulated by actual input, it undergoes decoherence and collapses to one of the ground states, resulting in a classical weight vector.

In comparison to classical neural networks, QNN offers notable advantages such as faster computation, larger memory capacity, smaller network size, and the avoidance of the catastrophic forgetting phenomenon. However, there are still obstacles to overcome with regards to QNN's parameter training and updating. Although back-propagation method can be effectively implemented on simulators, its execution on real quantum processing units is

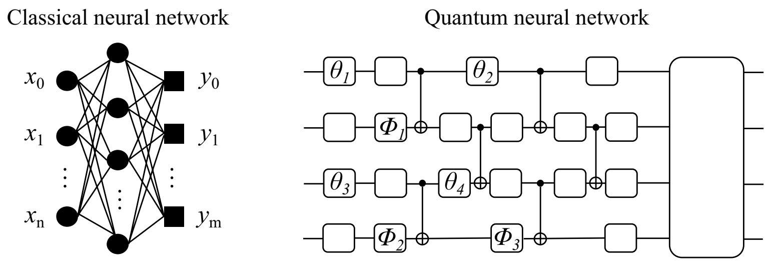


Fig. 14 Quantum control framework based on RL

a challenge (Melnikov et al. 2023). As such, an efficient alternative is needed and there is an expectation that the parameter-shift rule could provide a solution to address this issue.

It has been demonstrated that the quantum model (QM) could be expressed as a partial Fourier series in the statistics, wherein the available frequency is estimated by the data coding gate in the circuit. By reiterating uncomplicated data coding gates several times, QM can attain access to a progressively richer spectrum. A quantum model $f_\theta(x)$ is given by.

$$f_\theta(x) = \langle 0 \left| U^\dagger(x,\theta) M U(x,\theta) \right| 0 \rangle, \tag{5}$$

$$U(x) = W^{(L+1)} S(x) W^{(L)} \dots W^{(2)} S(x) W^{(1)}, \tag{6}$$

where x is an input vector, the quantum circuit $U(x,\theta)$ is dependent on the input vector x and a set of parameters θ, which may be void, M is the observable, $S(x)$ is the coding circuit for input vector x, $\left| 0 \right\rangle$ is the initial state, W is trainable circuit blocks and represents $W(\theta)$.

The initial step involves recognizing that an eigenvalue decomposition of the generator Hamiltonian $H = V^\dagger \Sigma V$ can always be obtained. Here, Σ is a diagonal operator with H's eigenvalues λ_1, λ_2, …,$\lambda_{d\text{-}1}$, λ_d positioned along its diagonal. Data encoding unitary $S(x)$ and data- dependent expressions of the quantum state $U(x) \left| 0 \right\rangle$ can be given by

$$S(x) = V^\dagger \mathrm{e}^{-ix\Sigma} V \tag{7}$$

$$\left[U(x)|0\rangle \right]_i = \sum_{j \in [d]^L} e^{-i\Lambda_j x} W^{(L+1)}_{ij_L} \dots W^{(1)}_{j_1 1} \tag{8}$$

where the notation $[d]^L$ represents any set of L integers chosen from 1,..., d, The aggregation of eigenvalues for a particular j can be represented as $\Lambda_j = \lambda_{j1} + \ldots + \lambda_{jL}$. Considered the complete quantum model derived from Eq. (5), it is necessary to consider the complex conjugation of the expression, as well as the dimension, resulting in the following equation:

$$f(x) = \sum_{k,j \in [d]^L} e^{i(\Lambda_k - \Lambda_j)x} a_{k,j} \tag{9}$$

$$a_{k,j} = \sum_{i,i'} (W^*)^{(1)}_{1k_1} (W^*)^{2}_{j_1 j_2} \dots \times W^{(2)}_{j_2 j_1} W^{(1)}_{j_1 1} \tag{10}$$

AII frequencies accessible to QNN are included in its spectrum and Eq. (9) can be further simplified as.

$$f(x) = \sum_{w \in \Omega} c_w e^{iwx}, \tag{11}$$

$$c_w = \sum_{\substack{k,j \in [d]^L \\ \Lambda_k - \Lambda_j = w}} a_{k,j}, \tag{12}$$

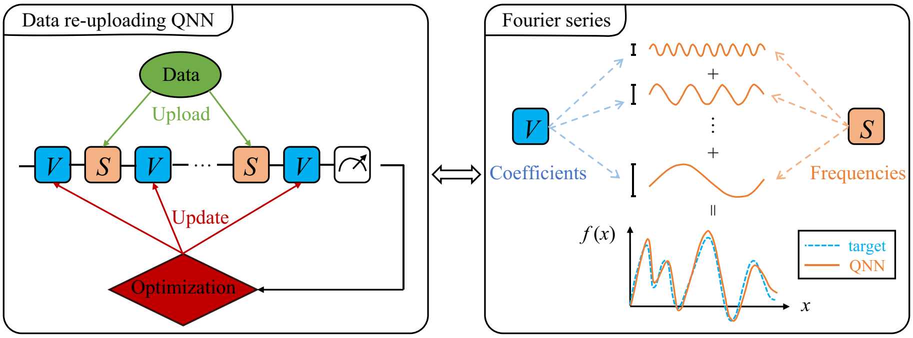


Fig. 15 **Data re-uploading QNN and Fourier series** (Yu, et al. 2022)

where $\Omega=\{\Lambda_k -\Lambda_j, k, j\in[d]^L\}$ denotes the discrete set of frequencies and cw can be obtained by aggregating all term subsidizing to the similar frequency.

Building upon the universal approximation property (UAP), Yu, et al. (2022) has shown that the coding block in the quantum network governs the range of the Fourier series, while the training block manages the Fourier measurements, as illustrated in Fig. 15. Moreover, it has been observed that approximating multivariate functions with single-qubit native QNNs may present certain challenges. However, Multi-qubit QNN requires exponential depth, which is unrealistic and does not contribute to the quantum advantage. The efficient implementation of QNNs that possess universal approximation properties for multivariate functions is an area of significant research interest.

4.2 Quantum gate

In both classical and quantum computing, gate operators are essential in manipulating data. While classical gates have the ability to convert inputs into outputs, quantum gates, in addition, permit input of superposition states and must satisfy some conditions such as reversibility. Among the various single qubit logic gates used in quantum computing, the Pauli gates, including X, Y, and Z, are widely employed. Specifically, the X gate rotates the quantum state corresponding to the x-axis of the Bloch sphere by an angle of π degrees. Similarly, the Y and Z gates rotate the quantum state by an angle of π degrees around the y and z-axis of the Bloch sphere, as illustrated in Fig. 16.

In quantum computing, data manipulation is heavily dependent on gate operators. Quantum gates, akin to classical gates, are responsible for transformation of inputs into

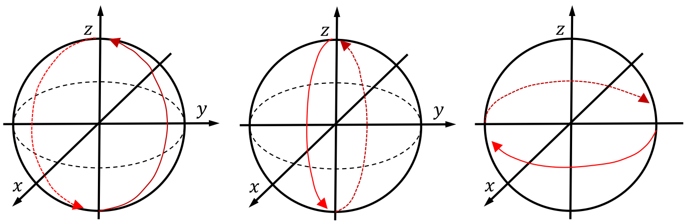


Fig. 16 Spin effect of Pauli gates

output states. Nonetheless, the quantum gates can manipulate input superposition states and adhere to specific principles, including reversibility. Among the frequently used single-qubit logic gates are X, Y, and Z gates, which are collectively known as Pauli gates. The X gate is responsible for flipping the ground state and serves as the quantum analogue of the classical NOT gate for non-superposed ground states. In addition to the Pauli gates, the S and T gates are also common single quantum logic gates. The S gate rotates the quantum state by 90 degrees around the z-axis of the Bloch sphere, while the T gate rotates it by 45 degrees. Furthermore, the H gate, or the Hadamard gate, is a fundamental quantum gate that finds widespread use in quantum circuits. It facilitates the transformation of the 0 or 1 state, expressible by classical computers, into the superposition state of $|+\rangle$ and $|-\rangle$, expressible solely by quantum computers. The relevant details of these single qubit logic gates are explained in the Table 1.

The quantum gates discussed above are suitable for single-bit operations, but to handle multiple bits, a multi-bit quantum gate, particularly the CNOT gate, is needed. The CNOT gate operates by entangling two qubits, with one of the qubits transformed into a superposition state using an H gate, and the second qubit being controlled by CNOT. However, other types of quantum gates that can connect multiple qubits also exist, as illustrated in Table 2. As the no. of qubits increases, the dimensionality of gate matrix also increases.

The utilization of well-known identity relationships to simplify circuits is highly advantageous. Through careful inspection, we can establish the validity of the following three identity relationships:

$$\mathrm{HXH} = \mathrm{Z} \tag{13}$$

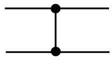
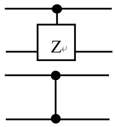
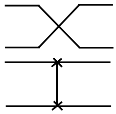
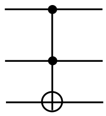
$$\mathrm{HYH} = -\mathrm{Y} \tag{14}$$

$$\mathrm{HZH} = \mathrm{X} \tag{15}$$

Table 1 Single-bit qubit gates

Operating symbol	Quamtum gate	Matrix
Pauli-X(X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-X(X)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-X(X)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard(H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase(S,P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
π/8(T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$

Table 2 Multi-bit qubit gates

Operating symbol	Quamtum gate	Matrix
Controlled-Not (CNOT, CX)		$\begin{bmatrix} 10 & 00 \\ 00 & 10 \\ 01 & 00 \\ 00 & 01 \end{bmatrix}$
Controlled Z(CZ)		$\begin{bmatrix} 10 & 00 \\ 00 & 10 \\ 01 & 00 \\ 00 & 01 \end{bmatrix}$
SWAP		$\begin{bmatrix} 10 & 00 \\ 00 & 10 \\ 01 & 00 \\ 00 & 01 \end{bmatrix}$
Toffoli (CCNOT,CCX,TOFF)		$\begin{bmatrix} 100 & 00000 \\ 010 & 00000 \\ 001 & 00000 \\ 000 & 10000 \\ 000 & 01000 \\ 000 & 00100 \\ 000 & 00001 \\ 000 & 00010 \end{bmatrix}$

4.3 Hybrid quantum neural networks

Numerous experiments and studies have demonstrated the superior classification and regression performance of hybrid quantum neural networks (HQNN) in comparison to classical neural networks. To illustrate, Perelshtein et al. (2022) designed a three-layer perceptron model and a hybrid quantum classical multilayer perceptron model. The HQC multilayer perceptron model shares the same last three layers as the three-layer perceptron model. The standard benchmark Scikit dataset (Perelshtein et al. 2022) was utilized to evaluate the models. The findings demonstrated that the hybrid quantum classical multilayer perceptron model achieved a classification precision of 13% higher than that of the three-layer perceptron model in test data, and its convergence speed was much faster. Furthermore, the classification accuracy of the hybrid model remained above 90% even after

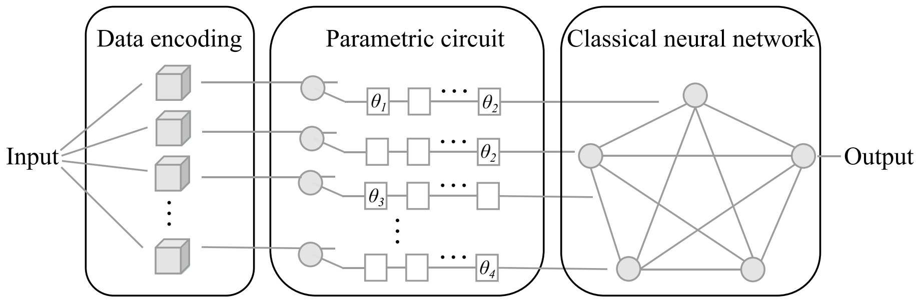


Fig. 17 General architecture of HQNN

reducing the size of the data used for training the model, whereas the learning ability of the classical model was significantly reduced. Similarly, in the case of the Boston housing dataset (Perelshtein et al. 2022), a three-layer perceptron model and a hybrid quantum classical multilayer perceptron model were used for the regression task. The lost values of the hybrid model were 12% higher than those of the classical model when the training set size was 400 and 16% higher when the training set size was 125.

Generally, the architecture of an HQNN comprises three components: data coding, quantum parameter circuit, and classical NN as depicted in Fig. 17. The encoder circuit is responsible for transforming classical data into quantum data. The middle quantum circuit is employed to optimize the attributes of the quantum gate. Finally, the classical NN executes the specific task.

The ability of a quantum ML model to represent data depends heavily on the data coding strategy employed (Schuld et al. 2021). A well-designed coding scheme can improve the efficiency of the model. To enhance the expressive power of quantum circuits, repeated coding strategies have been proposed to add more Fourier bases to the final functional representation (Schuld et al. 2021). In addition, a novel boson data coding scheme based on the use of photons has been proposed (Gan et al. 2022). This method employs a reduced number of coding layers to incorporate classical data points by associating data points with high-dimensional Fock space. The expressive power of the circuit can be effectively regulated by modifying the number of input photons. Quantum photonics offers exclusive benefits in enhancing the expressive potential of quantum ML models.

CNNs are widely used in classical ML and have been combined with quantum circuits to create hybrid models (Sebastianelli et al. 2021; Houssein et al. 2022; Liang et al. 2021; Hur et al. 2022). However, when a QNN is a confined quantum system, its dynamics are governed by unitary transformations. The residual scheme, which is commonly used in CNNs, will increase the trace of the input–output matrix, making it impractical for implementation on a quantum computer. To address this, (Liang et al. 2021) proposed a novel quantum–classical NN called Res-HQCNN, which improves the cost function of both clean as well as noisy quantum data. Res-HQCNN also incorporates the residual scheme into the feedforward QNN to modify the training procedure, particularly the process of updating the unitary perceptron. Experimental results showed that Res-HQCNN outperforms existing technologies in learning unknown single transformations and exhibits greater robustness to noisy data. These findings provide a valuable reference for future research on quantum residual learning.

Hybrid quantum neural technology has been extended to recurrent neural network (Elkenawy et al. 2021; Samuel et al. 2022; Ceschini et al. 2022), generative adversarial network (GAN) (Haozhen et al. 2023) and graph neural networks (GNN) (Ai et al. 2022). Elkenawy et al. (2021) proposes an observer based on a feedforward neural network to estimate the state of the confined system, and develops an adaptive control based on actor-critic to realize RL, using a quantum diagonal recurrent neural network (QDRNN) to denote the critical and actor portions. (Samuel et al. 2022) proposes a mixed quantum–classical model of LSTM and proves its successful learning on several time data, paving the way for the implementation of ML algorithms for sequence modeling, and its suitability for natural language processing and speech recognition. Quantum generative models (QGAN) have demonstrated superiority to classical GANs in theory or experiment. However, their practical application is hindered by the lack of physical qubits in existing quantum hardware, making it difficult to generate high-resolution images. Haozhen et al. (2023) proposes an image generation scheme using a GAN (HQCGAN) and remapping method, optimizing the structure of QGAN to minimize the number of attributes, without affecting the potential acceleration of the quantum algorithm. Ai et al. (2022) proposes a new hybrid quantum–classical algorithm for graph structure data, called the decomposed quantum graph NN, which realizes the theoretical framework of GNN by tensor product and identity matrix, and outperforms existing models with only 1.68% of parameters.

To address the issue of small sample size in specific applications, transfer learning (TL) has been widely applied to classical neural networks. The application of TL to HQNN has also shown great potential and received increasing attention. TL can alleviate the challenge of training with limited samples and improve training efficiency by leveraging the knowledge learned from relevant tasks. In this process, the network model that has been learned or trained from the relevant tasks is transferred to the model architecture of the new task, followed by optimizing only some final layers for specific tasks and interested data sets, as illustrated in Fig. 18. The well-known classical neural models including AlexNet (Krizhevsky et al. 2017), ResNet (He et al. 2016), Inception (Szegedy et al. 2015), Transformer (Vaswani et al. 2017) have been effectively trained.

Three new transfer learning (TL) variants have been proposed for hybrid quantum neural network (HQNN) in reference (Mari et al. 2020). The CQ variant transfers prior knowledge from a pre-trained conventional neural network to the classical network part of HQNN. QC and QQ variants use fixed quantum circuits as general quantum feature extractors for pre-training. CQ has been validated through a series of tests in references (Kim et al. 2022). In reference (Umer et al. 2022), a pre-trained ResNet-18 model is applied to the depth feature collection and provided as input to the 4-qubit quantum circuit. The model is trained on two publicly available X-ray imaging datasets with tuned hyper-parameters, achieving an accuracy index of 99.0%. CQ has also been verified in speech recognition as demonstrated in reference (Umer et al. 2022), where a pre-trained CNN network is transferred to a part of the HQNN model. Joint fine-tuning with the variations of quantum circuit (VQC) based on the Google voice command dataset showed that the hybrid TL algorithm of HQNN can improve the baseline performance on spoken command recognition tasks, as confirmed by the simulation results.

The vast majority of existing HQNN are still only simulated and validated on simulators due to the current limitations in physical quantum hardware. The number of qubits required for running these algorithms on real quantum devices is presently unattainable. One reason for this is the inadequate performance of the Noisy intermediate-scale quantum (NISQ) hardware. Research into NISQ hardware innovation is therefore a crucial area for future exploration. Additionally, mapping classical data to quantum data is just the starting point, and compressing classical data to facilitate effective representation

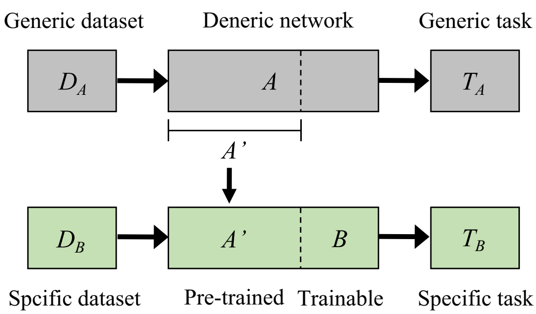


Fig. 18 Transfer learning

on real quantum devices is also an area that warrants further attention. Another important direction for future research is adjusting the no. of quantum bits and the depth of quantum circuits needed by the algorithm. In this regard, Matrix Product States and the corresponding quantum circuit methods might be a useful reference. Furthermore, the gradient vanishing phenomenon, generalization capability, over-fitting, over-parameterization, entanglement dropout, and small sample training of HQNN are all significant research directions for the future.

5 ethical implications and challenges for AI and quantum computing

5.1 Ethical implications for AI and quantum computing

As AI and quantum computing continue to advance and become more integrated into our daily lives, it is essential to consider the ethical implications that come with their use. One of the most pressing issues is data privacy and security. With the increasing amount of data being generated and collected, it becomes easier for bad actors to access sensitive information and use it for malicious purposes. This is where quantum computing comes in as it has the potential to break current encryption methods and make it easier for hackers to access data that was previously considered secure.

Furthermore, AI systems can also pose ethical concerns, particularly in the areas of bias and discrimination. If the data used to train these systems is biased, then the resulting AI algorithms will also be biased, leading to unfair treatment and discrimination against certain groups.

Another issue that arises with the use of AI and quantum computing is the potential for job displacement. As these technologies become more advanced, they will likely replace some human jobs, leading to economic disruption and social inequality. Therefore, it is crucial for researchers, policymakers, and stakeholders to work together to address these ethical concerns and ensure that the development and use of AI and quantum computing align with societal values and promote the greater good. This includes developing robust security and privacy measures, addressing bias and discrimination in AI systems, and creating policies that support a smooth transition for workers impacted by automation.

5.2 Challenges and limitations

There are several challenges and limitations associated with the convergence of AI and quantum technology. AI algorithms often require specialized processors such as Graphics Processing Units (GPUs), while quantum computers rely on qubits, which are currently difficult to scale and operate at extremely low temperatures. The integration of these two technologies requires hardware compatibility, which is currently a major challenge.

- *Software compatibility* The programming languages used for AI and quantum computing are also different. AI algorithms often use high-level programming languages such as Python, while quantum algorithms require low-level programming languages such as QASM. Integrating the two technologies requires software compatibility, which is also a challenge.

- *Noise and error correction* Quantum computing is prone to noise and errors due to the fragile nature of qubits. This means that quantum algorithms require error correction techniques, which can be computationally expensive. Integrating AI and quantum technology requires efficient error correction techniques that can mitigate the effects of noise and errors.
- *Limited resources* Current quantum computers have limited qubits and are unable to perform complex computations required for many AI tasks. This means that integrating AI and quantum technology requires the development of more powerful quantum computers.
- *Talent shortage* Finally, there is a significant shortage of experts who are skilled in both AI and quantum technology. The integration of these two fields requires experts who have a deep understanding of both technologies, which is currently rare.

6 Conclusions and outlook

AI for quantum refers to the application of AI techniques in developing quantum algorithms and the utilization of quantum computing to advance AI applications. The amalgamation of AI and quantum computing holds immense potential for yielding significant breakthroughs across diverse fields, including artificial intelligence. The convergence of AI and quantum computing presents vast possibilities for practical applications. Quantum computing is also leveraged to improve AI applications. For example, quantum computing can expedite NN training, a crucial component of machine learning. Moreover, quantum computing can aid in boosting the efficiency of optimization algorithms, commonly employed in AI applications. Currently, the development of quantum mechanics technology is limited, and there are no commercially viable quantum products available, such as quantum computing and quantum communication. Several physical underlying problems remain unsolved, and while conventional methods may seem theoretically feasible, their implementation is often inadequate. To usher in a commercial era of quantum technology, it is essential to address the many challenges in quantum mechanics. AI may prove to be a powerful tool in overcoming these obstacles and may facilitate the formulation of new physical experiments. Moving forward, there is an expectation to enhance the accuracy and resilience of ML algorithms in physical and quantum applications, as well as to develop new algorithms that are suitable for use in actual quantum physics experiments. Furthermore, QC can be used to unravel problems that are difficult for classical computers. These problems include optimization, pattern recognition, and natural language processing, among others. Therefore, the combination of AI and quantum computing can lead to significant breakthroughs in various fields, including drug discovery, finance, and cybersecurity.

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Declarations

Ethical approval Not applicable.

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