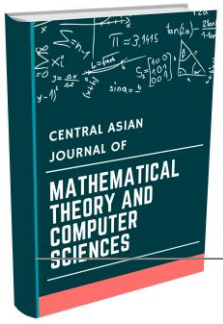

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SYNERGY BETWEEN QUANTUM COMPUTING AND MACHINE LEARNING IN QUANTUM NEURAL NETWORK

Sadia Rafi

School of Natural Sciences, National University of Sciences and Technology

sadiarafi012@gmail.com

Rana Muhammad Ali Maisam, Anum Zahid, Muhammad Haroon Yaqoob, Shoaib Ajmal

Department of Physics, COMSATS University Islamabad, Lahore, Pakistan

ranaalimaisam@gmail.com, anumzahid1998@gmail.com, Haroonyaqoob126@gmail.com, shoaibdasti11@gmail.com

Adnan Azam

Department of solid-state physics Punjab university

adnanazam251295@gmail.com

Abstract

Machine learning has made significant contributions to the fields of chemistry and materials science, enabling the exploration of vast chemical space through large-scale quantum chemical calculations. These models provide fast and accurate predictions of atomistic chemical properties, but they have limitations when it comes to capturing the electronic degrees of freedom of a molecule. This restricts their application in reactive chemistry and chemical analysis. To address this limitation, we introduce a deep learning framework that predicts the quantum mechanical wavefunction of a molecule in a local basis of atomic orbitals. The wavefunction serves as a foundational representation from which all other ground-state properties can be derived. Our approach maintains complete access to the electronic structure through the wavefunction, while achieving computational efficiency comparable to force-field methods. Moreover, the framework captures quantum mechanics in a form that can be analytically differentiated, allowing for efficient optimization and exploration of chemical systems.

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We demonstrate the potential of our approach through several examples. By leveraging the predicted wavefunction, we showcase the ability to perform inverse design of molecular structures to target specific electronic property optimizations. This opens exciting avenues for tailoring molecular structures to achieve desired electronic characteristics. Additionally, our framework paves the way for enhanced synergy between machine learning and quantum chemistry, enabling more comprehensive investigations into complex chemical systems.

Introduction

Machine learning (ML) methods have made significant progress in the field of quantum chemistry and materials simulation, particularly in the development of predictive models for interatomic potential energy surfaces. These potential energy surfaces play a crucial role in understanding the behavior and properties of molecules and materials at the atomic level.ML algorithms have the capability to capture complex relationships and patterns in large datasets, making them well-suited for modeling the potential energy surfaces. By training on quantum mechanical calculations and experimental data, ML models can learn the underlying physics and chemistry governing the interactions between atoms (Behler and Parrinello 2007, Braams and Bowman 2009, Bartók, Payne et al. 2010, Smith, Isayev et al. 2017) molecular forces, electron densities (Chmiela, Tkatchenko et al. 2017, Chmiela, Sauceda et al. 2018, Ryczko, Strubbe et al. 2019). Indeed, the availability of large data sets comprising molecular properties calculated from quantum chemistry simulations or measured from experimental studies has facilitated the construction of predictive models for exploring the vast chemical compound space. These data-driven models leverage machine learning and statistical techniques to establish correlations and patterns between molecular structures and their corresponding properties. By training on these extensive data sets, predictive models can learn the relationships between molecular features and properties, enabling the estimation or prediction of properties for new or unexplored compounds. This approach offers a powerful tool for screening and prioritizing compounds with desired properties, accelerating the discovery and optimization of materials for various applications. The integration of quantum chemistry calculations and experimental measurements in these data sets provides a comprehensive and diverse representation of the chemical compound space. Quantum chemistry calculations offer detailed insights into the electronic structure, energetics, and reactivity of molecules, while experimental measurements provide valuable information on physical, chemical, and biological properties. The construction of predictive models using these data sets involves various machine learning algorithms, such as regression, classification, or deep learning approaches. These models can capture complex relationships and non-linear dependencies between molecular features and properties, enabling accurate predictions and efficient exploration of chemical compound space (Rupp, Tkatchenko et al. 2012, Jha, Ward et al. 2018, Von Lilienfeld 2018). Recent research has delved into the potential of machine learning techniques in constructing approximate quantum chemical methods and predicting quantum chemical properties. One area of investigation focuses on developing machine learning models that can approximate the calculations of higher-level quantum chemical methods, such as MP2 (Møller-Plesset perturbation theory) and coupled cluster energies, using information from lower-level calculations based on Hartree-Fock orbitals. By leveraging large datasets consisting of quantum chemical calculations, machine learning algorithms can learn the underlying relationships between the lower-level and higher-level calculations. This enables the efficient estimation of more accurate energies without the need for computationally expensive calculations. In addition, there have been approaches that employ neural networks as a basis representation of the wavefunction. Traditionally, the wavefunction, which describes the quantum state of a system, is expressed using mathematical functions. However, by using neural networks, which are highly flexible and adaptable models capable of capturing complex patterns, researchers aim to represent the wavefunction in a more efficient and accurate manner. Neural network-based representations of the wavefunction have shown promise in capturing the intricate electronic structure and quantum mechanical behavior of molecules (Sugawara 2001, Carleo and Troyer 2017, Li, Collins et al. 2018, Welborn, Cheng et al. 2018, Cheng, Welborn et al. 2019). Most existing machine learning (ML) models in the field of quantum

chemistry have a common characteristic: they learn from quantum chemistry data to describe molecular properties as scalar, vector, or tensor fields. Scalar fields capture properties that have a single value associated with each point in space. Examples of scalar fields in quantum chemistry include atomic energies, molecular energies, electron densities, and atomic charges. ML models can learn the relationships between molecular structures and these scalar properties, enabling predictions of these properties for new or unexplored molecules (Grisafi, Wilkins et al. 2018).

2- The variational circuit structure of QNNs

Quantum neural networks (QNNs) typically employ parameterized quantum circuits, which encode variational parameters into rotation angles of specific quantum gates. These gates, including parameterized single-qubit rotation gates (Rx(θ), Ry(θ), and Rz(θ)), Controlled-NOT gates, and Controlled-Z gates, form the fundamental components of the quantum circuit ansatz. Together with the cost function ansatz and classical optimization strategy, these elements constitute the overall framework of a QNN The output of a quantum neural network (QNN) can be represented by the expectation values of certain measurements, denoted as Vi(θi), where Vi represents a variational quantum block with parameter θi. It is important to emphasize that in amplitude-encoding based QNNs, they can be considered as kernel methods, highlighting the significance of the data encoding approach (Boutet, Madhavan et al. 2021).

Quantum Machine Learning for Signal Processing

Quantum machine learning (QML) offers several advantages over classical machine learning approaches. Firstly, it has the potential for lower memory storage requirements. Quantum systems can efficiently represent and process information, allowing for more compact memory usage in QML models.Secondly, QML provides enhanced security for model parameters through encryption techniques based on quantum principles. Quantum encryption ensures secure communication channels, protecting sensitive information during training and inference processes (Mitarai, Negoro et al. 2018)

Furthermore, QML exhibits good feature representation capabilities. By leveraging quantum properties such as superposition and entanglement, QML algorithms can capture complex patterns and correlations in data, enabling richer feature representations compared to classical approaches.QML encompasses various variants that explore different aspects of quantum computing and machine learning. Adiabatic quantum computation (AQC) is one such variant, where a quantum system evolves from an initial state to a final state encoding the solution to a computational problem. AQC has been applied to optimization and machine learning tasks, such as clustering and classification.Another variant is quantum circuit learning (QCL), which utilizes parameterized quantum circuits as the learning model. The variational parameters in the quantum circuit are optimized to minimize a cost function, allowing the circuit to learn and make predictions. QCL has been employed in regression, classification, and generative modelling tasks (Havlíček, Córcoles et al. 2019)

Additionally, quantum kernel methods leverage quantum feature spaces and similarity measures for machine learning. These methods aim to exploit the unique properties of quantum systems to develop efficient and powerful learning algorithms. Quantum kernel methods have shown promise in support vector machines and kernel ridge regression. Quantum variational autoencoders (QVAEs) combine the principles of variational autoencoders with quantum circuit learning. QVAEs utilize quantum circuits to encode and decode data into latent representations, enabling generative modelling and data reconstruction tasks. These variants and advantages of QML highlight its potential to revolutionize machine learning by harnessing the power of quantum systems. Ongoing research and development in this field continue to explore new techniques and applications, paving the way for exciting advancements in AI (Farhi, Goldstone et al. 2000, Yang, Qi et al. 2021).

Quantum learning, in conjunction with decentralized speech processing, offers promising opportunities for innovation and advancement

While quantum technology is relatively new, attempts have been made to leverage it for speech processing. One such attempt was proposed by Li, who introduced a speech recognition system incorporating quantum

back-propagation (QBP) simulated by fuzzy logic computing. However, it should be noted that QBP does not directly utilize qubits in real-world quantum devices, and the approach fails to fully demonstrate the inherent quantum advantages of this computing scheme. Additionally, the complexity of the QBP solution poses challenges for large-scale automatic speech recognition (ASR) tasks, particularly in terms of parameter protection.From a system perspective, the advantages offered by quantum computing, such as encryption and randomized encoding, are highly desirable for federated learning systems, including distributed ASR. Cloud computing-based federated architectures have emerged as effective solutions for industrial applications, showcasing the quantum advantages using commercial NISQ (Noisy Intermediate-Scale Quantum) servers. These architectures enable the exploitation of quantum benefits within the context of federated learning, aligning with the requirements and demands of decentralized speech processing systems (Li, Zhao et al. 2002, Yang, Liu et al. 2019, Qi, Yang et al. 2020).

3- The design of quantum convolutional neural networks (QCNNs) tailored for speech recognition tasks is being explored

In recent research, a new approach called Quantum Convolutional Neural Networks (QCNN) was introduced, inspired by the idea of utilizing Variational Quantum Circuits (VQCs) as convolution filters with quantum kernels. The purpose of QCNN is to extend the properties of traditional Convolutional Neural Networks (CNNs) into the quantum domain, specifically for image processing tasks. One notable advantage of QCNN is its ability to construct convolution kernels using fewer qubits during the Quantum Machine Learning (QML) process. A QCNN is composed of multiple quantum convolutional filters, each responsible for transforming input data. To achieve this, a quantum circuit is designed, which can follow a structured or randomized approach. The quantum convolutional filter applies this circuit to the input data, leveraging the unique properties of quantum systems to perform the convolution operation. This allows QCNN to explore the potential benefits of quantum computation in image processing tasks, opening up new possibilities for quantum-enhanced machine learning (Henderson, Shakya et al. 2020).

To obtain the output of a quantum convolutional layer, the quantum convolutional filter comprises three key components: the encoding function (e(•)), the decoding operation (d(•)), and the quantum circuit (q(•)). The following steps outline the process:

Chunking: The 2D Mel-spectrogram input vectors are divided into smaller 2 × 2 patches. Each patch, indexed as 'n', undergoes encoding within the quantum circuit. This encoding step is represented as Ix[n] = e(ui[n]), where ui[n] represents the nth patch (Yang, Qi et al. 2021).

Quantum Circuit Operation: The initial quantum states, Ix[n], are processed through the quantum circuit using the operator q(•). The quantum circuit applies a series of quantum gates and transformations to the input states, resulting in transformed states. The output after applying the quantum circuit is denoted as Ox[n] = q(Ix[n]) (Yang, Qi et al. 2021)

Measurement: Since the outputs of the quantum circuit exist in a quantum state, they are measured to obtain classical information. This measurement involves projecting the qubits onto a set of quantum state bases that encompass all possible quantum states and operations. By measuring the quantum states, the desired output value, fx,n, is obtained as fx,n = d(Ox[n]). The decoding operation, d(•), extracts the relevant information from the measured quantum states, producing the final output value (Yang, Qi et al. 2021).

Undefined Quantum circuit

To ensure parameter protection in Quantum Convolutional Neural Networks (QCNN), a random quantum circuit is deployed, denoted as U, with a unique design generated for each QCNN model. This random quantum circuit consists of various quantum gates, including Rx, Ry, Rz, and CNOT. The classical input vectors are initially encoded into a quantum state $\Phi 0 = |0000\rangle$. The encoded quantum states undergo the following phases within the quantum circuit U:

Phase 1: $\Phi 1 = Ry|0\rangle\ Ry|0\rangle\ Ry|0\rangle\ Ry|0\rangle$

Phase 2: Φ2 = (RxRy|0〉)|CNOT(Ry|0〉)Ry|0〉 RzRy|0〉

Phase 3: Φ3 = CNOT((RxRy|0〉))CNOT(Ry|0〉)Ry|0〉 RzRy|0〉

Phase 4: Φ4 = RxRyΦ3

It is important to note that random quantum circuits may involve multiple CNOT gates, which can introduce noisy signals, especially in non-error-corrected quantum devices and considering the connectivity of physical qubits. To mitigate this issue, the number of qubits is limited to a small quantity, ensuring that the noise tolerance capabilities of Variational Quantum Circuits (VQCs) are not exceeded(Bergholm, Izaac et al. 2018).

For simulation purposes on a CPU, PennyLane, an open-source programming software for differentiable programming of quantum computers, is utilized to generate random quantum circuit. Additionally, the random quantum circuit is constructed using Qiskit, a software development kit for quantum computing, to simulate the noise models obtained from IBM quantum machines with 5 and 15 qubits, providing more advanced simulations beyond ideal noiseless scenarios (Henderson, Shakya et al. 2020, Yang, Qi et al. 2021).

Recurrent Neural Networks with Attention Mechanisms

We adopt a deep attention-based Recurrent Neural Network (RNN) model called RNNAtt as our baseline architecture for the local model, specifically for second-pass models in the Federated Learning (VFL) setting. RNNAtt consists of two layers of bi-directional Long Short-Term Memory (LSTM) units and incorporates a self-attention encoder \[27\]. This model, compared to other Deep Neural Network (DNN) solutions like DS-CNN and ResNet, has been reported to achieve the best results in spoken word recognition (Hochreiter and Schmidhuber 1997, De Andrade, Leo et al. 2018)

To ensure consistency in our experiments and reduce architectural variations, we conduct ablation studies. Additionally, we propose an advanced attention RNN model called RNNUAtt, which incorporates a U-Net encoder. The RNNUAtt model applies a series of multi-scale convolutional layers (with channel sizes of 8-16-8) to quantum-encoded (quanv) or neural convolution-encoded (conv) features. This approach aims to enhance the generalization of acoustic features by learning scale-free representations. Both RNNAtt and RNNUAtt models are used in our experiments to evaluate the advantages of utilizing the proposed Quantum Convolutional Neural Network (QCNN) model.In our local model, depicted in Figure 3 (b), we include a loss calculation layer on top of the RNN backbone. For spoken word recognition, we employ the cross-entropy loss for classification. In future studies, we may explore replacing the loss layer with connectionist temporal classification (CTC) loss for large-scale continuous speech recognition tasks (Warden 2018, Chen, Suresh et al. 2019, Raju, Filimonov et al. 2019).

Future Perspective and Conclusions

In this paper, we have introduced a novel approach to decentralized speech processing for vertical federated learning, leveraging quantum convolution for feature extraction. Our proposed Quantum Convolutional Neural Network (QCNN) models have demonstrated competitive performance in spoken-term recognition while ensuring model parameter protection and preserving interpretable acoustic feature learning. Notably, the QCNN models have exhibited stable performance when trained on quantum machines, outperforming classical Deep Neural Network (DNN) based Acoustic Model (AM) models with equivalent convolutional kernel sizes.Our future work will focus on integrating QCNN into continuous Automatic Speech Recognition (ASR) tasks. By doing so, we aim to explore the potential of QCNN models in improving the accuracy and efficiency of continuous speech recognition systems. Additionally, while our proposed VFL-based ASR architecture addresses data protection requirements by decentralizing prediction models, we acknowledge the importance of further enhancing privacy measures. To this end, we plan to incorporate additional statistical privacy measurements to strengthen the security and privacy aspects of the proposed QCNN models, considering other perspectives.

In conclusion, our research presents a promising direction for decentralized speech processing in vertical federated learning, providing a framework that combines the power of quantum convolution with effective feature extraction. The results obtained from the proposed QCNN models support their viability and competitiveness in spoken-term recognition tasks. We anticipate that our work will contribute to advancing the field of quantum-assisted machine learning and inspire further exploration of QCNN models in various speech processing applications.

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