Communication efficiency enhanced federated learning derived from quantum reinforcement learning for retrosynthesis

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***Abstract*—The combination of parametric quantum circuits and density matrix coding can significantly reduce the number of parameters in artificial neural networks. The reduction in the number of model parameters helps to improve the communication efficiency when training deep learning models under federated learning architectures. In this study, we showcase the enhanced communication efficiency achieved in federated learning by utilizing quantum neural networks in the context of the molecular inverse synthesis task within reinforcement learning. Specifically, we consider the federated learning task on the reinforcement learning-based retrosynthesis. we adopted the USPTO-50k chemical reaction dataset. the MLP and quantum neural network are used as the agent of the reinforcement learning algorithm, respectively. Enhancements in communication efficiency stem from the capacity of encoded quantum states within quantum neural networks to effectively represent data. All instances are additionally situated within the framework of ligand molecules associated with Tau proteins.**

***Index Terms*—federated learning, quantum machine learning, reinforcement learning, retrosynthesis**

I. Introduction

The increasing maturity of quantum computers has ushered in an era of novel computational tools. [1] The profound impact of quantum computing on drug design has garnered widespread attention. Among these quantum algorithms, we find UCCSD, which relies on the quantum phase estimation algorithms, quantum optimization solvers, and quantum machine learning techniques. [2] The fusion of quantum data advantages with deep learning tasks is poised to assume a pivotal role both presently and in the future. [3] Meanwhile, the application of deep learning in the field of biomedicine hinges upon the availability of high-quality datasets and the imperative of safeguarding data privacy. [4] Enter federated learning, a crucial approach in today's deep learning landscape for addressing data privacy concerns. Notably, this framework is also adaptable for quantum machine learning applications. [5]

In the realm of federated learning, the process of training deep learning models locally necessitates communication and updates with servers or other clients, adhering to algorithms like FedAvg. [6] As the data's feature encoding complexity grows, there is a consequential surge in the neural network's parameter count. This, in turn, amplifies the communication overhead associated with training deep learning models within federated learning frameworks. For federated learning to remain practical, it becomes imperative to discover means of substantially reducing model parameters while employing the same data preprocessing techniques, all without compromising model performance significantly. [7]–[9]

In this context, it's worth highlighting that quantum neural networks have the potential, under specific conditions, to yield such outcomes. An illustrative case in point is the realm of reinforcement learning applied to molecular inverse synthesis, as mentioned earlier. [10] Within the chemical industry, the plan-

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ning of chemical reaction pathways assumes paramount significance, particularly in the production of organic molecules. One notable approach, exemplified by Aspuru-Guzik et al., leverages reinforcement learning algorithms in tandem with chemical reaction templates. [11] In their work, the authors employed Multi-Layer Perceptrons (MLP) and molecular fingerprinting to craft an intelligent framework for decision-making regarding chemical reaction types. By subsequently converting the internal structure of this intelligent framework into parametric quantum circuits, a remarkable reduction in the number of parameters becomes evident. [12]–[14]

To explore the potential utility of quantum neural networks in the context of drug design, we delve into our work centered on small molecule targeted drug design for Tau proteins. [15] Our approach involves utilizing the open-source binding energy prediction model, deepDTA, to identify molecules with the highest affinity for Tau from the USPTO-50k chemical reaction database. [16] Subsequently, we employ a reinforcement learning/quantum reinforcement learning inverse synthesis strategy to dissect the synthetic pathways leading to the desired molecules. Throughout this process, we illustrate how quantum neural networks contribute to heightened communication efficiency when training reinforcement learning inverse synthesis algorithms within the framework of federated learning.

II. Methods

A. Quantum Neural Networks

The quantum neural network represents a fusion of neural network algorithms and quantum computing techniques. Neural network algorithms form the foundation, with implementations typically relying on PyTorch. Similarly, software frameworks for quantum computing, such as Qiskit, are predominantly Python-based. [17] In our work, we focus on parameterized quantum circuits, primarily employing quantum computing simulators. These parameterized quantum circuits serve as the building blocks for our neural networks, replacing traditional MLP (Multi-Layer Perceptron) networks responsible for decision-making in reinforcement learning algorithms.The optimization of our quantum neural network is accomplished through the Adam optimizer, featuring a loss function rooted in the L1-parameter implementation of measured and true values. The initial learning rate is set at 0.001.

The structure of the parameterized quantum circuit with N-bits is outlined as follows:

a Pauli-X gates with a phase rotating gate(phase parameter-1), Pauli-Y gates with a phase rotating gate (phase parameter-2), and Pauli-Y gates with a phase rotating gate (phase parameter-3) collectively compose the XYZ layer structure.

b Pauli-Y gates with a phase rotating gate(phase parameter-4), Pauli-Z gates with a phase rotating gate (phase parameter-5), Pauli-Y gates with a phase rotating gate (phase parameter-6), constituting the YZY layer structure.

c Pauli-Z gates with a phase rotating gate (phase parameter -7), Pauli-Y gates with a phase rotating gate (phase parameter -8), and Pauli-X gates with a phase rotating gate (phase parameter -9), constituting the ZYX layer structure.

d Pauli-X gates with a phase rotating gate (phase parameter -10), Pauli-Z gates with a phase rotating gate(phase parameter -11), Pauli-X gates with a phase rotating gate (phase parameter -12), constituting the XZX layer structure

e Pauli-Y gates with a phase rotating gate (phase parameter -13), Pauli-Z gates with a phase rotating gate (phase parameter -14), and Pauli-Y gates with a phase rotating gate (phase parameter -15), constituting the YZY layer structure.

f Adding the ring gates of Control-NOT between a and b, b and c, c and d, d and e without phase parameter.

B. Reinforcement Learning for Inverse Synthesis Design

Our analysis of chemical reaction inverse synthesis is based on the USPTO-50k open-source dataset. The algorithm for specifying chemical reaction pathways is derived from the reinforcement learning model detailed in Aspuru-Guzik et al.'s work. Our implementation of reinforcement learning relies on tools such as PyTorch and RDKit. [18], [19] Additionally, we introduce quantum reinforcement learning by substituting the Multi-Layer Perceptron (MLP) in the original algorithm with a quantum neural network. The algorithm unfolds as follows:

Data Preprocessing

- The chemical reaction data undergo an initial preprocessing step. They are organized into a chemical synthesis file, comprising product information, reaction categories, and synthetic details. The file adheres to the following data structure:{product1:{category1:[reactant1, reactant1, reactant1...], category2:[reactant1, reactant1, reactant1...] ...}}.
- We utilize the RDKit chemoinformatics tool to generate a Morgan fingerprint for each molecule. Furthermore, we label attributes indicating whether each molecule is a target product and its purchase availability.
- The data structure of Tree is employed to manage the reverse search process of chemical reactions. In this structure, the root node corresponds to the initial level labeled as 1, and the highest level of the tree is capped at 10, representing the maximum reaction steps. The root node holds the "target product" molecule, while branch nodes store intermediates, leaf nodes signify terminal points, and synthetics molecules populate the structure.

Model Training:

- The RDKit chemical information tool was employed to generate the Morgan fingerprint for each molecule. Additionally, attributes indicating whether a molecule is a target product and its availability for purchase were labeled.
- The search for synthetic paths leading to target products was carried out using recurrent learning, with the result-

ing path data structured into a Tree Data Structure and stored in the experience pool. Data from the experience pool also plays a role in computing loss functions for neural networks and quantum neural networks.
- The molecular fingerprint data obtained from RDKit must be encoded in compliance with the constraints of the quantum state density matrix. Once encoded, it is utilized to estimate the loss value when fed into the quantum neural network.
- Upon algorithm convergence, inputting target product molecules yields locally optimal chemical reaction pathways structured within a tree-data structure.

C. Federated Learning

Federated learning is a machine learning paradigm that prioritizes data privacy by keeping training data local while facilitating global model training through the sharing of model gradients. Our work leverages the FedAvg algorithm, which follows this process: [20]

1 Initialize the global neural network model on a central server.
2 Distribute the global model to each participant.
3 Each device independently trains the model using its local dataset and generates a gradient update for the model.
4 Transmit the gradient updates from each device back to the central server.
5 The central server aggregates model updates from all devices and computes their average.
6 The central server then returns the average to each device for updating their local model.

These steps (3-6) are iteratively executed until the global model converges or reaches a predetermined number of iterations.

D. Virtual Screening Model

In our research, we employed a deep learning model for predicting the strength of Tau interactions with small molecules and for filtering target molecules from the USPTO-50k dataset, drawing inspiration from the open-source work, DeepDTA. To adapt the model to our needs, we retrained it using the PBDbind dataset. We transformed the inputs, represented as SMILES, into vectors using dictionaries and utilized embedding vectors to project these vectors into a higher-dimensional space. This preprocessing step optimized the input data for ligands, enhancing computational efficiency.For processing sequence data, we followed a similar approach. [21]

In our virtual screening model, we constructed a DeepDTA network model, incorporating a convolutional neural network (Conv1d), a linear layer, and a ReLU activation function. The preprocessed ligand SMILES and receptor data served as inputs, processed in batches. To minimize the error between predicted and true values, we employed the Mean Squared Error (MSE) loss function. The Adam optimizer was utilized to fine-tune the model parameters, reducing errors and enhancing model fit. During the training process, we set a learning rate of 0.001, ran 600 epochs, and processed 32 samples per batch. These parameters were carefully chosen to facilitate gradual learning of input data characteristics and to incrementally improve prediction accuracy. Through diligent training and optimization, we successfully developed a regression model tailored for ligand-receptor interactions.

III. Results and Discussion

A. Workflow

Federated Quantum Reinforcement Learning for Synthesis Path Planning of Targeted Drugs for Tau Proteins is presented in Figure 11. Our research hinges on the USPTO-50k chemical reaction template database, where we conducted training for both quantum reinforcement learning and reinforcement learning for reverse synthetic path analysis. Additionally, we introduced federated learning to safeguard the security of chemical reaction data.

Furthermore, we harnessed this deepDTA model to predict the interaction strength between Tau proteins and targeted small molecules. Quantum reinforcement learning and reinforcement learning models were employed to meticulously craft optimal reaction pathways for these targeted small molecules.

In this comprehensive workflow, we independently implemented quantum reinforcement learning, federated retrosynthesis algorithms, and applied these models to dissect the synthetic pathways of ligand molecules for Tau proteins.

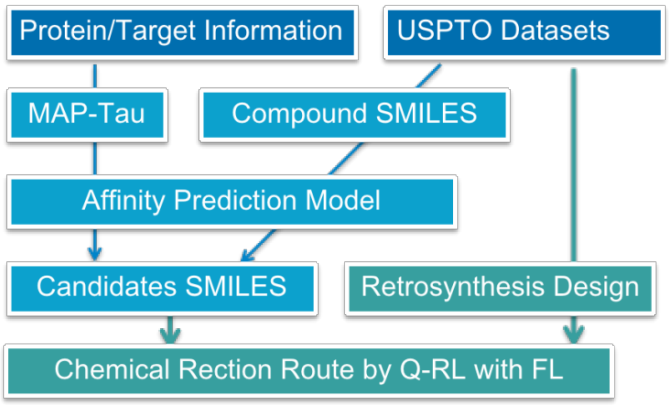
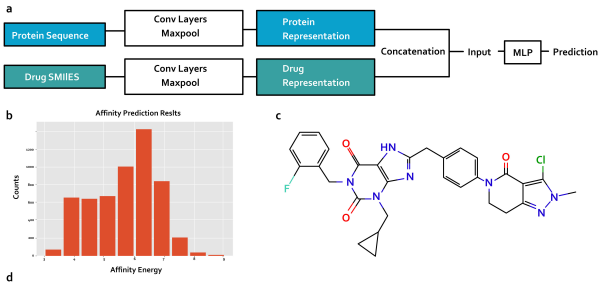


Fig. 1. Federated quantum reinforcement learning workflow for retrosynthesis of ligand Molecules targeting the Tau protein.

B. Screening candidates for the microtubule-associated protein Tau

G. Lee et al. provided essential information about tau protein and its significance in neurobiology and Alzheimer's disease, which provides a foundation for further research and exploration of this protein's functions and roles in health and disease. [15] To screen candidate targeting small molecules from the database of uspto-50k, we used the open-source DeepDTA model that is developed by Elif Ozkirimli et. al. As shown in Fig. 2a, this method first uses Conv1d to extract features from protein sequences and small molecule

SMILES coding, and employs an aggregation network to predict binding energies. Specifically, we retrained the DeepDTA model using the PDBbind dataset. It completed convergence after 300 epochs. We used the model to analyse the affinity energy values between Tau and ligand molecules. These ligand molecules are from uspto-50k datasets. In Fig. 2b, we have represented the distribution of affinity energies of drug molecules in bar degrees. Among them, We selected the molecule that has the largest value of binding energy with Tau. The chemical structure of this molecule was shown in Fig. 2c. We assessed the drug-like properties of molecules via MolWt (molecular weight), BertzCT (molecular complexity index), TPSA (molecular polar surface area), LogP (Wildman-Crippen LogP value71), and NumHAcceptors (number of hydrogen acceptors). These proprties were calculated with RDkit. In subsequent stages, we intend to leverage the trained reinforcement learning model to generate synthetic paths.



d

MolWt	BertzCT	TPSA	LogP	NumHA
590.06	1950.73	110.81	4.05	8

Fig. 2. Ligand molecule screening for Tau proteins. a. predictive modeling of affinity energy using convolutional neural networks and multilayer perceptronic (MLP) Neural Networks; b. statistical distribution of affinity between Tau proteins and small molecules in the USPTO-50K dataset; c. chemical structural formula of the screened molecules; d. the molecular weight, molecular complexity index, molecular polar surface area, Wildman-Crippen LogP value, and number of hydrogen acceptors of molecules.

C. Reinforcement Learning Algorithms for Chemical Retrosynthesis

We have developed an inverse synthesis algorithm for chemical reaction path planning using reaction template data sourced from the USPTO-50k dataset. Our reinforcement learning inverse synthesis algorithm draws inspiration from prior works. This reinforcement learning-based retrosynthetic model, utilizing the reaction template database, incorporates molecular fingerprints and information on the purchasability of molecules for synthetic path planning.

As shown in Fig. 3a, a neural network is employed to predict the reaction type, and this information is deposited into the experience pool (Buffer). The neural network parameters are continuously updated using data from the reaction database. The algorithmic flow is described in the Methods section. Besides, we have replaced this MLP neural network (Fig. 3c) with a quantum neural network (Fig. 3b). In our quantum neural network, the density matrix of this quantum state is determined through the Hermitian matrix calculation, which is related to structural information of the molecule. The visual depiction of the quantum circuits in our quantum neural network can be observed in Fig. 3b, illustrating each layer comprising rotation operators of Pauli gates and controlled operators. For constructing the loss function, we rely on the final state following quantum state evolution and its corresponding measured values. Throughout the reinforcement learning training process, our quantum neural network continuously adjusts the learnable phase information. At the present stage, quantum neural networks are executed within a quantum simulator environment.

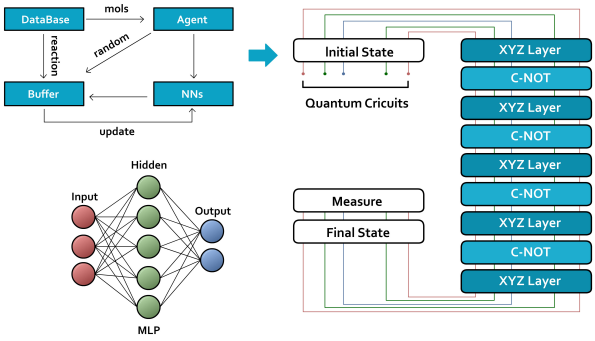


Fig. 3. Quantum reinforcement learning (QRL). a. reinforcement learning for retrosynthesis; b. quantum neural network as the agent; c. MLP as the agent.

D. Quantum information processing boosts communication efficiency

Considering the commercial value and privacy concerns surrounding chemical reaction datasets, we implemented federated learning to safeguard their privacy. Figure 4 illustrates our approach about Federated Quantum Reinforcement Learning (FQRL). Introducing quantum neural networks into privacy-preserving federated learning leads to enhancements in communication efficiency. Communication between server and client come from the exchange of the parameter of agent neural network.

We distribute the chemical reaction template data across various clients, and the neural network, along with the initial model parameters, is transmitted from the central server to these clients. We've chosen the FedAvg algorithm for training the neural network and updating parameters within the federated learning framework. Similarly, quantum neural networks have been integrated into this federated learning workflow.

In our approach, molecules undergoing processing are assigned a molecular feature vector using the ECFP fingerprint, resulting in a vector of length $F = 255$. This vector, along with the depth value of the reaction path, collectively generates a 256-bit molecular features. Subsequently, following the quantum information processing procedure, we derive a 8-qubit input quantum state for the parameterized quantum circuits, considering $log(F) = log256 = 8$. The number of

parameters in an MLP algorithm, which employs an input-hidden-output layer structure, is chiefly determined by input features and the dimensions of the hidden and output layers. However, employing the same molecular description vector with the density matrix of a 8-bit quantum state obtained after quantum information processing significantly reduces the number of parameters in the quantum neural network.

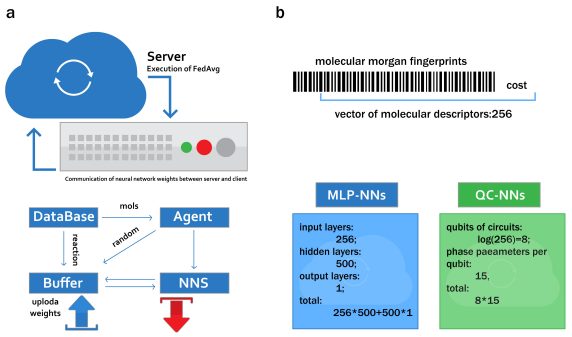


Fig. 4. Federated Quantum Reinforcement Learning (FQRL). a. communitation between the server and client; b. comparison of parameters between MLP and quantum neural network.

While the quantum neural network effectively reduces its parameter count to address the same task, it demonstrates the capability to execute the training task within the federated learning framework. We were able to find a comparison between Federated Reinforcement Learning(FRL) and Federated Quantum Reinforcement Learning(FQRL) in the Fig. 5a. Due to the decreased parameters in the quantum neural network, the communication between the server and the client per round is now only 0.1 percent of its previous value. Simultaneously, we conducted synthetic route planning for molecules exhibiting the highest affinity energy values predicted by DeepDTA, with the results depicted in Fig. 5c. To further understand the retrosynthesis in Fig. 5., DFT calculations by ORCA 5.0.1 [22] at B3LYP [23]–[25] /def2-SVP [26] level of theory conjunction with the SMD [27] continuum solvation model in the solvent of Chlorobenzene and Grimme's D3 [28]–[30] dispersion corrections were performed. The calculations show the reaction is exothermic by 7.5 kcal mol-1, confirming the reaction is favorable thermodynamically.

We have been investigating the performance improvements achievable in quantum machine learning applications. Quantum reinforcement learning, exemplified by its communication efficiency gains in federated learning, stands out as a positive outcome. However, it's important to note that not all quantum machine learning tasks exhibit comparable results, as the reduction in the number of parameters may be impacted by model convergence. Furthermore, the training of federated reinforcement learning, characterized by changes in algorithmic logic and update strategy, experienced some efficiency degradation compared to reinforcement learning training. We aim to address and enhance these aspects in our future work

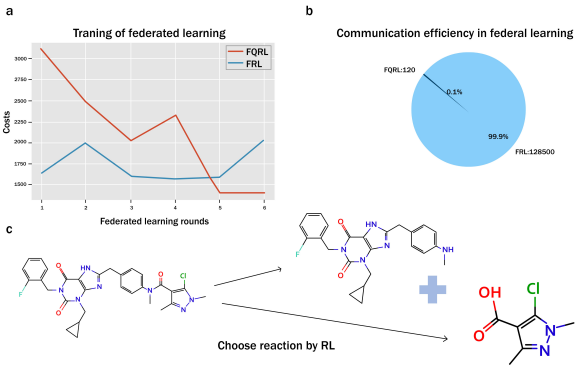


Fig. 5. The communication efficiency of federated retrosynthesis. a. the training of FQRL and FRL; b. comparison of communication costs between FQRL and FRL; c. Synthesis path given by reinforcement learning.

IV. Conclusion

In our study, we introduce quantum information processing to enhance the privacy-preserving capabilities of reinforcement learning inverse synthesis algorithms. Our implementation of the quantum reinforcement learning algorithm successfully accomplishes the task of reverse synthesis of chemical reactions while substantially reducing the parameter load in server-client communication for federated learning.

Our exploration of the potential of quantum machine learning is particularly profound within the context of molecular design of ligands for Tau proteins. This endeavor not only furthers our understanding of quantum machine learning but also delves into its real-world applicability, serving both academic and industrial interests.

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