Letter of Intent

Machine Learning and Architectural Perspectives for Quantum HEP Applications

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Abstract

We are exploring quantum computing technology, aiming to advance our understanding in fundamental science including high-energy physics at colliders. Our main interest is to promote applications of quantum technologies to realize large-scale "quantum artificial intelligence", potentially being a transformative technology in fundamental science. In the present LOI, we focus on quantum machine learning and near-term quantum architecture that will enhance quantum computing applications to high-energy physics.

1 Quantum Machine Learning for HEP

Quantum Machine Learning (QML) is considered to be a promising early quantum computing application in the Noisy-Intermediate Scale Quantum (NISQ) era [1]. One of the near-term QML architectures is Variational Quantum Algorithm or VQA (see e.g., Ref. [2] for review). In VQA, input classical data $\boldsymbol{x}$ are encoded into a Hilbert space with unitary $U(x_i)$, creating a quantum state $|\phi(x_i)\rangle = U(x_i)|0\rangle^{\otimes n}$ where n is the number of qubits. The $|\phi(x_i)\rangle$ is then processed using parametrized quantum circuit (PQC) $V(\boldsymbol{\theta})$ with tunable parameters $\boldsymbol{\theta}$. The processed state $|\psi(x_i, \boldsymbol{\theta})\rangle = V(\boldsymbol{\theta})|\phi(x_i)\rangle$, called ansatz, is measured with certain observables to quantify the objective function, which is then minimized to perform a desired task such as classification, regression or optimization. This architecture allows us to construct a shallow quantum circuit suitable for NISQ devices.

1.1 Machine Learning with Enhanced Data Encoding

The early VQA-based studies in HEP, such as the classification of physics process of interest from Standard Model background processes (e.g., Ref. [3,4]), are largely based on the encoding of input data using single-qubit rotation gates or ZZ-type interaction gates. These encoding schemes do not depend on the data type, therefore expected to work well for a wide range of input data. However, they are rather arbitrary, and generally require a large number of gates or qubits to encode multi-dimensional data, hence may not be optimal for HEP applications.

We propose to investigate more advanced data encodings suitable for large-scale, high-dimensional data in HEP. They would include the data re-uploading architecture with trainable

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embedding [5], error-robust encoding [6] and quantum random access coding [7]. The proposal aims to get insights for encoding scheme that scales efficiently with the input data size, enhancing the overall VQA performance in the combination with PQC.

1.2 Optimization Landscape in Variational Algorithm

A key question for VQA is whether it can be superior to classical machine learning in terms of learnability and generalizability with NISQ device. When the parameters $\boldsymbol{\theta}$ are optimized by minimizing the objective function, it is known that the optimization process often results in a vanishing gradient, called "Barren Plateau" [8]. More precisely, for sufficiently expressive ansatz (i.e., unitary 2-design ansatz), the gradient of the objective function vanishes exponentially with the number of qubits. This could be a fundamental bottleneck in VQA that prevents us from reaching advantage over classical machine learning in the training step. Furthermore, it is known that this problem arises not only in gradient-based optimizers but also in gradient-free optimizers [9], and quantum noise can cause similar effects [10].

The Barren Plateau depends on the type and depth of ansatz, so it would be important to numerically and analytically study the effects, aiming to clarify how and when such problem occurs. The proposed research aims to investigate efficient circuit design that mitigates the Barren Plateau phenomena. We plan to explore such design for specific ansatz relevant for Quantum Field Theory (QFT) simulations.

2 Near-Term Quantum Architecture for HEP

Encoding a quantum algorithm into a quantum circuit and executing it, under hardware constraints on qubit counts, connectivities and coherence times, are crucial steps for making the best use of near-term quantum devices. We propose to approach this "circuit optimization and execution" task for HEP applications from three directions.

2.1 Circuit Transpilation Protocol

The proposed research aims to extend the quantum circuit optimization protocol called AQCEL [11]. Two separate ideas constitute the implementation of the current AQCEL protocol: recognition of repeated patterns of quantum gates, and reduction of quantum gates with the identification of computational basis states. The novel functionality of AQCEL resides in the optimization performed on quantum device using polynomial computational resources.

The AQCEL optimization is deployed on a quantum algorithm for parton shower simulation, demonstrating a drastic reduction of the circuit length while maintaining the computational accuracy. We propose to extend the AQCEL protocol with optimized control/synthesis of "all microwave"-based quantum gates for near-term devices, including the possibility of using higher-energy states for information storage.

2.2 Pseudo-Quantum Memory

One of the biggest hurdles in the current quantum computing technology is the absence of "Quantum Memory" (QM), i.e., a mechanism for long-term storage of the state of quantum registers. Without QM, it is often the case that the encoding part of input data consumes a significant portion of the coherence time, leaving little time for actual algorithm to process the data. The

QM is an active field of research, but its realization has significant technical and fundamental challenges to overcome.

We are exploring methods to approximately store the state of a quantum computer. Our proposal is to utilize a short PQC $U(\boldsymbol{\theta})$ to "uncompute" the state (i.e., restore the initial state) of a quantum computer at a given point in the quantum circuit. VQAs are employed to find the set of parameter values that minimizes the distance between the uncomputed and initial states. Once the optimal parameters $\boldsymbol{\theta}^*$ are identified, the inverse of the uncomputing circuit $U^\dagger(\boldsymbol{\theta}^*)$ can be used to approximately reconstruct the quantum state created by the original circuit. In this sense, the circuit and the parameter values serve as 'pseudo'-quantum memory. We are exploring the usability over quantum states created by QFT simulations.

2.3 Custom Gate Operation for HEP

Universal gate sets provide a finite length of gate sequence that approximates any quantum operation with a given precision (Solovay-Kitaev theorem). Consequently, circuit composers can calibrate a finite set of single- and two-qubit gates, called "basis gates", and build their algorithm expressed with a sequence of the basis gates. Such calibrations are performed on a regular basis in backends of the Cloud-based superconducting qubit systems. In addition, users can construct "customized gates" by scheduling user-defined drive waveforms to each qubit. By using open-source software (e.g., Qiskit Pulse [12]), we can develop customized gates and include them in our basis gates to accelerate the operation of HEP-oriented quantum circuits.

The proposed research includes such middleware development to expand the capabilities of quantum processors, for example by making special two-qubit gates and methods to benchmark them. We are investigating this approach to improve the implementation of multi-controlled gates, e.g., Toffoli gate [13], which are ubiquitous operations for quantum HEP simulation and reconstruction algorithms.

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