Towards the Scalable Quantum Machine Learning for High-Energy Physics

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1 Quantum Machine Learning Opportunities on HEP community

High energy physics (HEP) community faces one of biggest data and simulation challenges on energy, intensity and cosmology frontiers. The data challenges will be expected to be much significant due to new instruments such as DUNE (Deep Underground Neurino Experiments), High Luminosity LHC (Large Hardon Collider), and LSST (Large Synoptic Survey Telescope) to list few and simulations of n-body and QCD simulations. Therefore, we need a scalability breakthrough on HEP in both training and inference. Quantum Computer (QC) is an ideal solution for this scalability challenge as it has the potential to achieve **exponential speed-ups** and revolutionize the way we handle the data.

Another aspect is that machine learning (ML), including deep learning (DL), has been demonstrated across HEP communities to be effective from event classification to galaxy deblending [1] and the trends would favor wider and more aggressive adoption in next decades. However, there are several opportunities to develop AI/ML in quantum computers:

- **Easier to develop and use Quantum Machine Learning (QML)**: there are entrance barriers in using and developing quantum machine learning models for HEP applications
- **Auto-tuning Quantum Machine Learning models**: Any machine learning model is required to tune hyper parameters and quantum machine learning is no exception.
- **Gaps in classical machine learning and quantum machine learning**: The quantum version of machine learning is in infancy status and there are a lot of opportunities to further develop quantum computer specialize algorithm developments.
- **Integration of Quantum Sensing, Internet, and Analysis**: Experimental HEP can be significantly benefited by quantum sensing as it can observe entangled states and such states can be transferred through quantum Internet to be analyzed by quantum computers.

2 HEP Quantum Machine Learning Strategies

Quantum machine learning models by HEP scientists With the recent advances in quantum machine learning, particularly the hybrid quantum-classical paradigm, several promising results has been demonstrated [2, 3]. However, such models need to be built with components from both the classical and quantum worlds. It is a non-trivial task for HEP scientists to construct these hybrid models in a reasonable effort. Our team has been working on a software framework to address these issues. The main features are 1) Collecting well-performed quantum circuits blocks. 2) Unified interfaces for users to define new quantum circuit architectures. 3) Highly reusable components. 4) Support for a wide range of quantum simulation backends and hardware. For the simulation part, it is desirable if we can use high-performance computing infrastructure to parallelize the quantum circuit simulation. 5) Integration with existing classical machine learning frameworks. For example, the data format and the gradient information should be compatible with the common deep learning frameworks.

Tuning the QML models After coming up with a hybrid quantum-classical architecture, it is often required to tune the hyperparameters for better performances. The search space for these hyperparameters can be intractably large which can only be resolved by the approximate optimization methods. Such *hyperparameter optimization* procedures, although studied extensively in classical machine learning community [4], to our best knowledge, has not been addressed much in the quantum machine learning community. Therefore, it is desirable to have a tool set to bridge the concept from classical ML into the quantum domain. For example, it is possible to incorporate the Bayesian methods in the optimization routine or it is also possible to treat the optimization as a black-box model and train a reinforcement learning (RL) agent to find the optimal hyperparameters.

Quantum Deep Learning In the recent decade, classical deep learning (DL) has been developed tremendously. A variety of architectures have been proposed and reached state-of-the-art performance. However, the quantum counterpart of these well-performing classical learning architectures are still unknown on quantum computing world. For instance, in computer vision, one of the major fields in classical machine learning, has largely depended the convolutional neural networks (CNN), which are also used in the high-energy physics widely. To tackle the coming high-dimensional high-volume data, it is promising to study the potential advantages to develop quantum deep learning algorithms including quantum CNN offered by quantum computers.

Quantum Sensing, Internet and Analysis together Quantum sensing is a promising direction of the research as it captures the entangled states directly and there are several experimental physics in HEP. The more opportunities are the combined power of quantum Internet and quantum computer together. One of the success of AI/ML is rooted from computing capabilities, algorithms and data together. HEP communities will find great benefits if we consider quantum sensing and Internet together on the quantum computing strategies as the current quantum Internet has been actively developing along with quantum sensing technologies.

References

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