NISQ Quantum Machine Learning for High Energy Physics*

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Motivation: High energy physics (HEP) is a scientific field that delves into the fundamental nature of our universe, studying particles and their interactions at the mist microscopic scales. As researchers strive to uncover new phenomena and push the boundaries of our understanding, vast amounts of data are generated by particle accelerators and detectors. Analyzing this data, and simulating unseen phenomena and interactions with particle detectors demands sophisticated computational techniques capable of extracting meaningful insights from complex datasets and is a promising application area for quantum machine learning (QML) [1].

Introduction: The application of QML in HEP data analysis holds tremendous potential for several reasons. First, and foremost, quantum computing harnesses the principles of quantum mechanics to perform computations in ways that classical computers cannot achieve efficiently. Combining this quantum computational power with machine learning algorithms unlocks new avenues for extracting valuable information from large-scale and complex HEP datasets [2, 3]. This capability can greatly enhance the analysis of high-dimensional datasets and enable researchers to uncover hidden patterns and correlations that might otherwise remain obscured. Secondly, HEP experiments often involve a multitude of parameters that influence the behavior and characteristics of particles and the simulation of their interaction at production and while interacting with the detector. QML algorithms can exploit the quantum nature of particles and the entanglement between them, enabling more effective parameter optimization and feature selection. Furthermore, QML offers the potential for learning the underlying physical interactions of a given system through the parameterization of a probability distribution from which new samples can be generated, accurately modeling complex physical systems. By simulating the behavior of particles and their interactions in a computationally efficient fashion, researchers can gain insights into the underlying physics, explore new theoretical models, and even optimize the design and performance of particle detectors and accelerators.

The potential impact of QML on HEP data analysis is increasingly recognized by researchers worldwide [4–10]. There is also the potential for HEP data analysis to benefit QML studies. The size of datasets, the complexity of the underlying problems, and the flexibility in feature selection provides a valuable source of real world data and applications that can either be mapped onto quantum models and circuits of limited width and depth or the data and scope can be used to push the state of the art in quantum model size and complexity. This is valuable in addressing the gap in the understanding the utility of NISQ devices for tasks with practical application in HEP workflows, as well as the scalability of such models beyond what can be simulated classically, and the impact of noise in model training and performance. A deep characterization of these models in terms of trainability, generalization, and expressivity is still needed, and several tools from the classical machine learning can be borrowed.

This abstract summarizes results from several studies that apply QML to HEP applications. The results are used to address several challenges associated with the adaptation of QML for data analysis tasks in HEP. By examining the ongoing research efforts and potential benefits, we aim to highlight the importance of QML in advancing our understanding of the fundamental nature of our universe and propelling HEP into a new era of discovery.

Quantum Generative models: Quantum unitary operations can effectively manipulate and modify distributions with shallow circuits. This can revolutionize data analysis in HEP by providing new ways to generate realistic and informative samples from complex distributions. Furthermore, quantum generative models can uncover latent patterns and structures in HEP datasets through unsupervised learning. By learning the underlying probability distribution of the data, these models can identify anomalies or rare events that deviate from the expected behavior. This capability is particularly valuable in HEP, where rare signals can indicate the presence of new particles or physics beyond the standard model. QML techniques can also be useful in sampling from complex distributions. HEP datasets often exhibit complex and high-dimensional probability distributions, making it challenging to sample from them efficiently. Furthermore, in some cases, integrals associated with the probability of a quantum particle being found at a specific position are hard to compute, due to the sign problem that plagues Monte Carlo calculations [11]. Quantum circuit Born machines (QCBM) can learn the underlying distribution of the data and generate new samples from it, or

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approximate the area under a complex function to be integrated. These generated samples can be used to augment training datasets, perform hypothesis testing, or explore regions of the distribution that are sparsely populated in the real data. These techniques leverage the power of quantum computers to model and simulate quantum systems, enabling the generation of samples that capture the underlying physics of HEP datasets.

Fitting Correlated Variables: In Ref. [12], we trained several QCBMs using gradient-based optimization to simulate the outcomes of particle collisions in proton-proton collisions, as seen from a typical detector at the Large Hadron Collider (LHC). These synthetic datasets accurately model the quantum behavior of particles and their interactions, and quantum generative models can generate models that provide insights into the underlying physics and help validate theoretical predictions. This can assist understanding background processes in particle detectors and identifying signals of new phenomena.

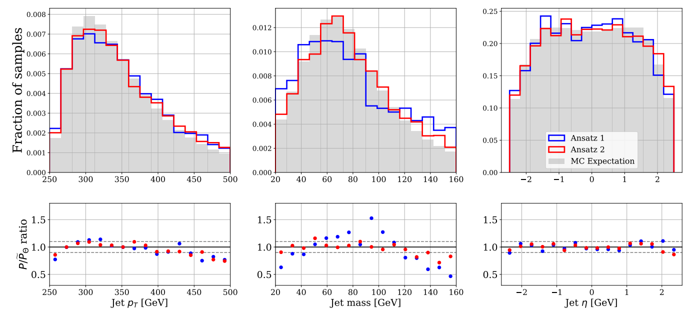

FIG. 1. Recovery of 3 marginal distributions from a QCBM trained with 12 qubits. (From Ref. [12]).

We demonstrated that QCBMs can be used to fit arbitrary joint distributions, and that these trained models can reproduce global behavior, local behavior and arbitrary correlations. To find a global model, the loss minimized during training compares the distance between the prepared joint distribution to the target. To verify that local models can be extracted, we demonstrated that by tracing over qubit subsystems we can reproduce the marginal probability distributions with high fidelity. Finally, we demonstrate that with an appropriate choice of ansatz, we can recover the correlations between the joint distributions. While it is possible to achieve any of these models individually, we found that circuits with denser entangling layers performed better at fitting local marginals, but the hardware efficient ansatz (HEA) performed the best overall with fitting all three models (global, local and recovering correlations).

Overparameterization: The models in Ref. [12] showed that QCBMs can be trained on $\geq$ 10 qubits and with several hundred parameters. This motivated a follow on study about the limitations of QCBMs in terms of width, depth and impact on trainability. We present empirical results on the onset of overparameterization in QCBMs. Overparameterization is a unique phase transition in the learning dynamics of neural networks which give counter-intuitive results. Overparameterization can lead to models with good generalization behavior instead of over-fitting, and we observe that overparameterized QCBMs train efficiently and effectively without impedance due to barren plateaus. We analyzed the training performance of QCBMs with different with and evaluate the training with respect to: a uniform distribution, a correlated two-dimensional joint distribution (HEP) generated from a Monte Carlo dataset of the simulation of a typical LHC proton-proton interaction, and a GHZ state. We identify a critical circuit depth associated with a sharp drop in the final Jensen Shannon Divergence (JSD) value (see Fig. 2). This transition has been associated with regions of over and underparameterized circuits, as quantified by the rank saturation of the Quantum Fisher Information (QFI), which coincides with the parameter dimension $D_C = 2^{n_{qubits}+1} - 2$, and in some cases, with the dimension of the Dynamical Lie Algebra associated with the generators of the circuit ansatz. Our findings indicate that these parameters act as a (loose) upper and lower bound for the onset of the trainability transition.

Quantum Generative Adversarial Networks: Quantum generative models based on adversarial training of two parameterized circuits can be trained to learn the background distribution from a process of interest, a signal or a rare interaction, from the background. In particular, machine learning models that include a generator and a discriminator component, can be used to determine whether a given event in an HEP dataset is characteristic for the learnt distribution. In this study, we explre the suitability of an unsupervised QML approach based on a quantum implementation of a generative adversarial network (qGAN). Our QML model features a quantum generator, and a quantum discriminator that is trained from classically encoded samples. The trained generator is used to construct an anomaly score that is used to determine the likelihood of a given sample of being an anomaly.

Supervised Learning: Another learning paradigm uses labeled samples and parameterized quantum circuits as classifier models. These have been explored in HEP in the context of event classification [9, 13], jet identification, and anomaly detection [7]. The applicability of QML models for anomaly detection in HEP is an exciting and potentially transformative area of research. In HEP experiments, the vast amount of data produced by experiments, like those conducted at the LHC, often contains rare or anomalous events that could signal new physics.

Understanding how to efficiently embed these datasets into quantum models could lead to major breakthroughs in our understanding of fundamental physics, allowing us to detect anomalies that could be indicative of previously unknown particles or interactions. We explore how different embedding techniques can enhance classification power for signal extraction in datasets where the noise to signal ratio is very high. QML models,leverage the power of quantum computing to handle high-dimensional data and model complex distributions, potentially enhancing the detection capability for these rare events.

Noise robustness: The study of hardware noise effects is of paramount importance due to the inherently fragility an sensitivity of quantum systems. Understanding these hardware noise effects helps in developing effective error correction and mitigation strategies. The effects of noise on a model's performance has been approached from several directions. Noise can be considered analytically [14, 15] and used to infer robustness of different model designs. Robustness can be experimentally qualified by training a model in noiseless simulation then further training on near-term hardware.

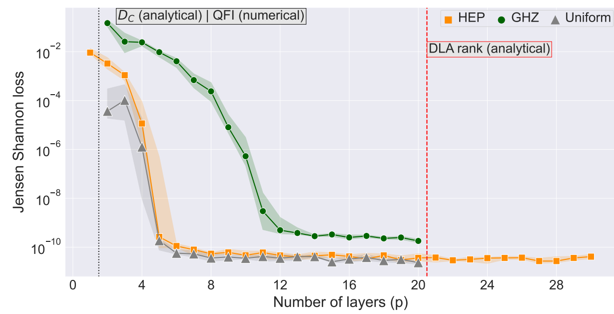

FIG. 2. Median (markers) and IQR (shaded) of final losses obtained over 100 QCBM training runs($N = 4$) as a function of the number of layers. Dashed and dotted vertical lines correspond to overparameterization bounds found in the literature.

We use the second approach to evaluate the robustness of QCBMs and quantum classifier models. where we adjust the parameter probabilities of depolarizing noise and bitflip noise as we train our circuit. The main idea was to mimic noise present during training on near-term quantum hardware, and to evaluate the resiliency of the quantum models. Our quantum classifier model has three main components: the feature embedding, the trainable unitary, and the measurement. Each component plays an important role on how well these models' classification power. Efficient circuits can utilize the entire Hilbert space to make for more robust and clear linear separations and classifications of our data. To this effect, we performed an extensive numerical study on noise robustness for quantum classifiers, as well as on the effect of several measurement settings.

Summary: This survey targets the widespread application of quantum machine learning in HEP data analysis tasks, where precise and reliable classifications are required. The development and adaptation of QML techniques for HEP data analysis fosters interdisciplinary collaboration between quantum scientists, machine learning experts, and high energy physicists. This collaboration allows for cross-pollination of ideas, methodologies, and insights, leading to breakthroughs in both quantum computing and particle physics.

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