Quantum Machine Learning concepts and applications

Abstract

We explore Machine Learning techniques and Quantum Computing concepts that could be applied in High Energy Physics considering a phenomenological and theoretical view. In this framework, we show the main tools to explore the Standard Model extensions, decay process and the parameter space. With this set of tools, we want to explore the bounds and define exclusion regions, this results might be interesting for the next generation of colliders and could prove to be useful in the understanding of phenomena.

1 Introduction

We recently find different literature about Artificial Intelligence, Machine Learning, Quantum Computing, Quantum Information and Quantum Machine learning, among other interesting and related topics [1, 2]. Besides, ideas and concepts coming from those areas are implemented in different environments: Finance, Cryptography, medicine, chemistry and social sciences; however, some concepts are unclear, in this document we want to discuss basic ideas behind those topics focusing on the mathematics, physics and computing. This document reviews ideas behind Quantum Computing, Machine Learning and Computing what are relevant for theoretical or phenomenological physicists with experience in High Energy Physics and with interests in technological topics. In this paper we talk about algorithms, Qubits, particles, matrices, standard model and new physics, classical and quantum Information whose are interesting topics for undergraduate and postgraduate students linked to the recent technological concepts [3]. In this paper, we want to explore literature, documentation and basic implementation, following the formalism highlight for the particle physics.

2 Materials, Models and Methods

Most of the literature provide relevant information on models and methods, which is important for understanding the procedures and models. However, in this document we are discussing about concepts related to Quantum Computing, Machine Learning, Quantum Machine Learning whose are outstanding for the physicists. In particular, we prepare some examples to show the fundamental concepts coming from physics and mathematics.

2.1 Machine Learning in HEP

Machine learning is shown to have plenty of use cases in the field of high energy physics [4, 5] such as the discovery of exotic particles, understand the underlying structure of matter, analyzing the behavior of different particles and classification of various particles based on their properties. Particle physics is an area where the density of data needed for analysis or simulation is quite large. This combined with the fact that the particles exhibit quantum mechanical behavior makes quantum machine learning a more suitable method than classical approaches. Simulation of quantum mechanical systems can be done much more efficiently using a native quantum computer. Quantum Machine Learning algorithms can be roughly divided into supervised and unsupervised learning algorithms.

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2.2 Supervised Learning

Supervised Learning technique require labels to predict an unknown variable of a new data point. The quantum support vector machine, quantum boltzmann machine, quantum neural networks are some of the algorithms that can be classified as supervised.

A support vector machine is an algorithm that finds a separating hyperplane between two classes of data points. This hyperplane can be in the original feature space or a higher-dimensional kernel space. The time complexity of this algorithm is $O(\log(\epsilon^{-1})poly(N, M))$. The quantum support vector machine (QSVM) can perform this task with a time complexity of $O(\log NM)$ since a quantum computer can perform inner product calculation using the properties of superposition. In a classification problem where particles are to be divided into two different sets (e.g. fermions, bosons. couplings or others) the QSVM can take in a large feature space and perform the task with higher efficiency [6, 7].

The Boltzmann machine is a type of recurrent neural network that is based on the Hopfield Network. The network architecture is quite simple consisting of two layers namely the visible nodes and the hidden nodes. Each node from both the layers is connecting to every other node in the network. It is also called an energy based model (EBM) since the Hamiltonian is used to define the network. Since the boltzmann machine is inherently a physics based model of computation, a better representation is proposed using a quantum computer. The restricted boltzmann machine is one of the most popular algorithms known for recommendation systems The quantum Boltzmann machine has shown some promise of outperforming classical boltzmann machines in predictive tasks [8].

2.3 Unsupervised Learning

Unsupervised Learning (UL) usually deals with clustering and generation of new data points. The quantum k-means algorithm and quantum GAN are the proposed algorithms in this section.

The K-means algorithm is used to divide an unlabelled dataset of points into clusters based on a distance metric (eg euclidean distance). The means which are also the centroids of cluster are usually initialized at random and the distance between the centroids and each data point is calculated. The running time of this algorithm $O(kdN)$ where n is the number of entities to be clustered and k and d are the number of clusters and the dimensions respectively. In the quantum k-means algorithm the euclidean distance calculation is done using a quantum superposition [9, 10]. Hence the quantum k-means algorithm is theoretically shown to be computationally more efficient. This is very useful if clustering needs to be done on particle physics datasets containing millions of records.

A GAN (Generative Adversarial Network) is an algorithm that is trained in a supervised fashion to generate unsupervised data [11]. It uses two competing neural networks called the generator and discriminator to perform a variety of classification and denoising tasks. A Quantum GAN was first proposed in ref. [12]. A quantum GAN would not only be capable of performing supervised classification tasks but also generate new data that is in accordance with the dynamics of a quantum system.

2.3.1 Beyond Standard Model

The Higgs observation by CMS and ATLAS at CERN support the SM as a framework to describe the interactions among particles at scale $\mathcal{O}(10^2 \text{ GeV})$. This model has been tested by CERN and LEP with successful results. Currently, the technological development allows the exploration through the computer: Simulations, high performance, big data, artificial intelligence, among others. In this work, we will focus on implementations for the theoretical and phenomenological researchers in HEP topics.

The evolution on calculation techniques and the new software tools allow to probe the SM (and its extended models) and the experimental results. In fact machine learning (ML) becomes one of the most interesting and powerful set of techniques and tools (sometimes called paradigm) for investigating the phenomena regarding experimental and theoretical High Energy Physics (HEP).

In this view, we can use Machine Learning and Quantum algorithms for:

- obtain a deep insights,

- recognize unknown patterns and
- create high perform predictive models from data.

In this paradigm there are different learning types: Supervised, such as regression and classification; and unsupervised, implemented to find a pattern more than prediction.

UL is focused on data with missing labels. One could ask, why do I need unknown data? In fact, data can be analyzed and classified in order to find some patterns. UL algorithms can be explore the data set and return clustering data and more. This is very atractive for experimentalist with data coming from colliders, surveys or big laboratories with relevant data base.

UL has been one technique implemented to search for new physics [13].

In HEP the ML can be implemented in a theoretical and experimental view:

1. Higher order computational methods: OneLoop, QCDLoop, LoopTools; parton level generators NNLO, DYNNLO, N3LO [4, 5]
2. Monte Carlo event generators and deep inelastic inclusive cross-sections: MadGrap, POWHEG and HERA [4, 14]

In the theoretical and phenomelogical view, researchers face on some challenges to implement this ML paradigm for scrutinizing the models and the theory, however in ref. [15] shows an application in a beyond standard model with new neutral gauge boson but it is toy model. Actually in ref. [16] is shown an interesting analysis to $t\bar{t} \to W^+ bW^- \bar{b}$ looking at the physical parameters as mass.

In this work we want to explore some models and implement novel techniques to investigate the behavior of the physical parameters for Two-Higgs Doublet model (THDM), new gauge group or other models related with new physics. In particular we focus on THDM-II and III types.

We expose some models to study using ML. In particular we write down the Lagrangian for the THDM type III because we want to explore the flavor-changing parameters. In a general way, the Yukawa sector for the THDM-III is given by [17]

$$
\begin{aligned}
\mathcal{L}_n^{THDM-III} &= \frac{g}{2}\left(\frac{m_i}{m_W}\right)\bar{d}_i\left[\frac{\cos\alpha}{\cos\beta}\delta_{ij}+\frac{\sqrt{2}\sin(\alpha-\beta)}{g\cos\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^d\right)_{ij}\right]d_j H^0 \\
&+ \frac{g}{2}\left(\frac{m_j}{m_W}\right)\bar{d}_i\left[-\frac{\sin\alpha}{\cos\beta}\delta_{ij}+\frac{\sqrt{2}\cos(\alpha-\beta)}{g\cos\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^d\right)_{ij}\right]d_j h^0 \\
&+ \frac{ig}{2}\left(\frac{m_i}{m_W}\right)\bar{d}_i\left[-\tan\beta\delta_{ij}+\frac{\sqrt{2}}{g\cos\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^d\right)_{ij}\right]\gamma^5 d_j A^0 \\
&+ \frac{g}{2}\left(\frac{m_i}{m_W}\right)\bar{u}_i\left[\frac{\sin\alpha}{\sin\beta}\delta_{ij}+\frac{\sqrt{2}\sin(\alpha-\beta)}{g\sin\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^u\right)_{ij}\right]u_j H^0 \\
&+ \frac{g}{2}\left(\frac{m_u}{m_W}\right)\bar{u}_i\left[-\frac{\cos\alpha}{\sin\beta}\delta_{ij}+\frac{\sqrt{2}\cos(\alpha-\beta)}{g\sin\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^u\right)_{ij}\right]u_j h^0 \\
&+ \frac{ig}{2}\left(\frac{m_u}{m_W}\right)\bar{u}_i\left[-\cot\beta\delta_{ij}+\frac{\sqrt{2}}{g\sin\beta}\left(\frac{m_W}{m_i}\right)\left(\tilde{Y}_2^u\right)_{ij}\right]\gamma^5 u_j A^0. \qquad (1)
\end{aligned}
$$

where $\left(\tilde{Y}_2^u\right)_{ij}$ are some of parameters that we could study in the ML paradigm. As we will show this kind of model may have a special general potential depending on, λ_i parameters and different relations between the scalar fields, Φ_1 and Φ_2 [18].

3 Discussion

In this document, we want to expose some concepts and ideas for the HEP-researchers with high interest in computing and technology that could be implemented in the model exploration or analysis of parameter space.

This is work is going on, and we hope to show results and implementations in the next stage. HEP needs more tools to improve run time, storage or processing of information; and the next generation of physicists must be update and improve their skills on new models and tools.

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