Quantum vs Classical Machine Learning for Vector Boson Scattering Background Reduction at the Large Hadron Collider

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Acknowledgments & Collaborators

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The Large Hadron Collider

The largest particle accelerator in the world

~8.6 km diameter ring ~100 m below Geneva

P. Higgs at the Compact Muon Solenoid (CMS)
The Big Data challenge at LHC

- LHC produces huge amount of data, coming from 40 million p-p collisions/second, producing PB/hour data streams at each detector, requiring sophisticated computing tools.

The World LHC Computational Grid (WLCG) project...
- ~1.4M cores, ~1.5 EB storage, from 170 sites in 42 countries.
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The World LHC Computational Grid (WLCG) project...
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- Machine Learning (ML) tools are becoming increasingly relevant in different aspects, but particularly to select the targeted events from the background of other highly probable and indistinguishable events

The Vector Boson Scattering

Generic Feynman diagram from p-p collision and involving vector boson scattering (VBS), with possible products

Covarelli, Pellen, Zaro, arxiv:2102.10991 (2021)
Signal vs background events

- some VBS events contributing to signal:

![Signal Diagrams]

- possible non-VBS events contributing to background:

![Background Diagrams]

Covarelli, Pellen, Zaro, arxiv:2102.10991 (2021)
Simulated data set (CMS collaboration)

- VBS events used in this work were generated with MadGraph5_aMC@NLO (Montecarlo generator fully developer within the CMS collaboration)

- CMS detector simulated with Geant4
Simulated data set (CMS collaboration)

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- Background events generated with either MadGraph or Phantom, taking into account the known ratio between different processes (1/10^4 is the signal/background occurrence)

<table>
<thead>
<tr>
<th>Process</th>
<th>XS (pb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Segnale</td>
<td></td>
</tr>
<tr>
<td>VBS</td>
<td>2.2</td>
</tr>
<tr>
<td>W+jets</td>
<td>6.1 \times 10^4</td>
</tr>
<tr>
<td>WW</td>
<td>114.7</td>
</tr>
<tr>
<td>ZZ</td>
<td>16.5</td>
</tr>
<tr>
<td>Top</td>
<td>974</td>
</tr>
</tbody>
</table>
Variables selection

- The variables chosen for the training are selected by looking at the ones with the largest differences between statistical distributions of signal and background.

(a) Azimuth angle of lepton (8)
Machine Learning

ML is based on finding suitable mathematical models (functions) mapping input data into output predictions.
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E.g., support vector machines (SVM)

E.g., deep neural networks (DNN)

Supervised learning by DNN

- Image classification after DNN training

In general:

ML task is to learn how \( f \) maps \( x \) into \( y \), on varying \( \theta \), such that the algorithm will correctly predict \( y \) upon being fed with a previously unknown \( x \).
Classical ML tools in this work

- DNN training with a set of labelled background and signal events

- minimization of cost function to find optimal weights

- performance is tested against un-labelled data

Typically between 5000 and 50000 nodes.
Quantum computing models for artificial neural networks

(a) Classical Neural Networks
(b) Quantum Neural Networks
(c) Quantum Perceptrons
(d) Quantum Kernel Methods
(e) Quantum Convolutional Neural Networks
(f) Dissipative Quantum Neural Networks

Mangini, Tacchino, Gerace, Bajoni, Macchiavello, EPL 134, 10002 (2021)
Quantum neural networks as parametrized quantum circuits

- in general: hybrid quantum/classical algorithms

Benedetti et al., Quant. Sci. Tech 4, 043001 (2019)

- specifically in this work

\[ x \rightarrow \text{vector of input variables} \quad \text{w} \rightarrow \text{parameters optimized during training} \]
Quantum circuits for VBS QML

- encoding variables (each variable on a qubit)

\[ |0\rangle \xrightarrow{U_{\text{map}}(x)} |0\rangle \quad \xrightarrow{R_x(\arcsin(x_0)) \quad R_z(\arccos(x_0^2))} |0\rangle \]

\[ |0\rangle \xrightarrow{} |0\rangle \quad \xrightarrow{R_x(\arcsin(\sqrt{x_1})) \quad R_z(\arccos(x_1))} |0\rangle \]

\[ |0\rangle \xrightarrow{} |0\rangle \quad \xrightarrow{R_x(\arcsin(\sqrt{x_2})) \quad R_z(\arccos(x_2))} |0\rangle \]

- variational quantum operation

\[ U_{\text{var}}(w) \xrightarrow{} R_x(w_0) \quad R_z(w_1) \quad U_{\text{ent}} \quad R_x(w_6) \quad R_z(w_7) \]

\[ R_x(w_2) \quad R_z(w_3) \quad R_x(w_4) \quad R_z(w_5) \quad R_x(w_8) \quad R_z(w_9) \quad R_x(w_{10}) \quad R_z(w_{11}) \]

\[ \times 2 \]

with

\[ U_{\text{ent}}(w) \xrightarrow{} H \]
Deriving and minimizing the Loss f.

- from the qubits measurements to the classification function
  
  e.g. on two qubits
  
  \[ p_{signal} \equiv \frac{e^{\bar{z}_0}}{e^{\bar{z}_0} + e^{\bar{z}_1}} \]
  
  \[ p_{background} \equiv \frac{e^{\bar{z}_1}}{e^{\bar{z}_0} + e^{\bar{z}_1}} \]
  
  where \( \bar{z}_0 \) and \( \bar{z}_1 \) are averaged over 8192 measurements on \( \sigma_z \) basis

- Loss function is built by the distance between the output function \( p_{signal} \) and the ideal classifier (giving results 1 for signal and 0 for background)

  \[ L_w(x, \theta, w) = \sum_{i=1}^{N} P(x_i) \log \left( \frac{P(x_i)}{Q(x_i)} \right) w_i \]

  Generalized Kullback-Leibler (KL) divergence for \( N \) qubits

- Minimization allows to find \( w_{opt} \)
IBM Quantum processors

Microwave electronics

Chip Board

5-qubit NISQ devices →

ibmq_belem

ibmq_5_yorktown
Results I: The Receiver Operating Characteristic (ROC) curve

- The classification performance is assessed by ...

\[ TPR = \frac{TP}{TP + FN} \]
\[ FPR = \frac{FP}{FP + TN} \]

**TPR**: probability of positive event to be correctly classified

**FPR**: probability of negative event to be classified as positive

Cugini, Gerace, Govoni, Perego, Valsecchi, submitted (2022)
Results II: Area under the ROC curve (AUC)

Classical vs Quantum ML as a function of number of variables used in the classification

Cugini, Gerace, Govoni, Perego, Valsecchi, submitted (2022)
Results III: AUC vs number of training events

Classical vs Quantum ML as a function of the number of events in the training set

Cugini, Gerace, Govoni, Perego, Valsecchi, submitted (2022)
QML for HEP event reconstruction: Notable examples with similar conclusions

- Event classification of SUSY data set using PQC
  
  Terashi et al., Comp. Soft. Big Sci. 5, 2 (2021)

- QML study of background reduction for $t\bar{t}H$ process at LHC
  
Summary

- QML via parametrized quantum circuits successfully applied to signal vs background classification for VBS simulated data from CMS

- Comparison between classical and quantum ML performances:
  1) QML reaches comparable performance to DNN for a much smaller number of events in the training set, for the same number of variables;
  2) A limited number of variables is sufficient to reach good classifier performances for QML algorithm

- Relevant for practical applications of NISQ devices in HEP, following recent trends within CERN that is massively interested in Quantum Computing applications
What next?

- Test on new IBM Q devices, as well as on different Quantum Computing platforms
- Training and test on the same quantum hardware
- QML on real CMS (or ATLAS) data sets
- Increasing number of qubits (variables over which training is performed) to compare classical and quantum ML in conditions where classical ML performs very well
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