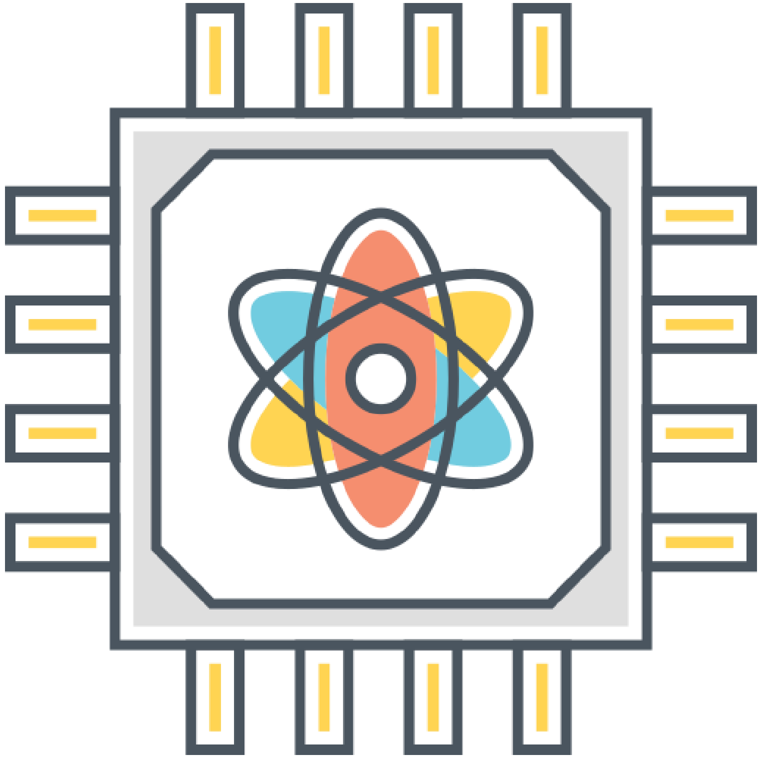
LIP LABORATÓRIO DE INSTRUMENTAÇÃO E FÍSICA EXPERIMENTAL DE PARTÍCULAS

Universidade do Minho

Quantum Machine Learning Applied to HEP: a Pragmatic Approach



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INTRODUCTION

SM AND BSM

Standard Model of Particle Physics (SM)

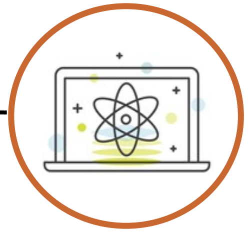
The Standard Model of Particle Physics (SM) has been highly successful in describing the fundamental constituents of matter and their interactions, as evidenced by its agreement with collider data.

Physics Beyond the Standard Model (BSM)

Nevertheless, **crucial questions persist**, such as gravity, dark matter, dark energy, and matter-antimatter asymmetry in the universe, **motivating** the **search for new physics beyond the SM** at the Large Hadron Collider at CERN.

QML IN THE CONTEXT OF BSM SEARCH

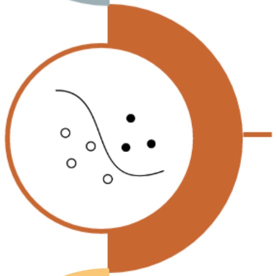
The exploration of BSM phenomena at colliders presents **challenges** due to **vast datasets** and **low signal-to-background ratios**.



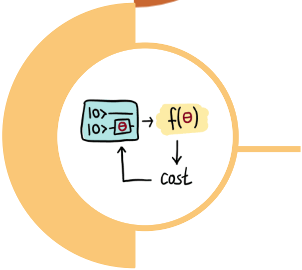
To tackle this **ML techniques**, particularly for **classification tasks**, have been employed, revealing their remarkable ability to **identify correlations** in **high-dimensional parameter** spaces.

PROJECT DEVELOPED

A systematic **comparison** is made between the **performance** of Quantum Machine Learning (**QML**) and shallow Classical Machine Learning (**CML**).



The primary focus is on **binary classification** tasks, specifically **distinguishing** between **BSM signals** and **SM background**.



The investigation involves the utilization of **VQC**s, while also **exploring the potential of reduced data** through feature reduction techniques.

VARIATIONAL QUANTUM CLASSIER

VARIATIONAL QUANTUM CLASSIFIER (VQC)

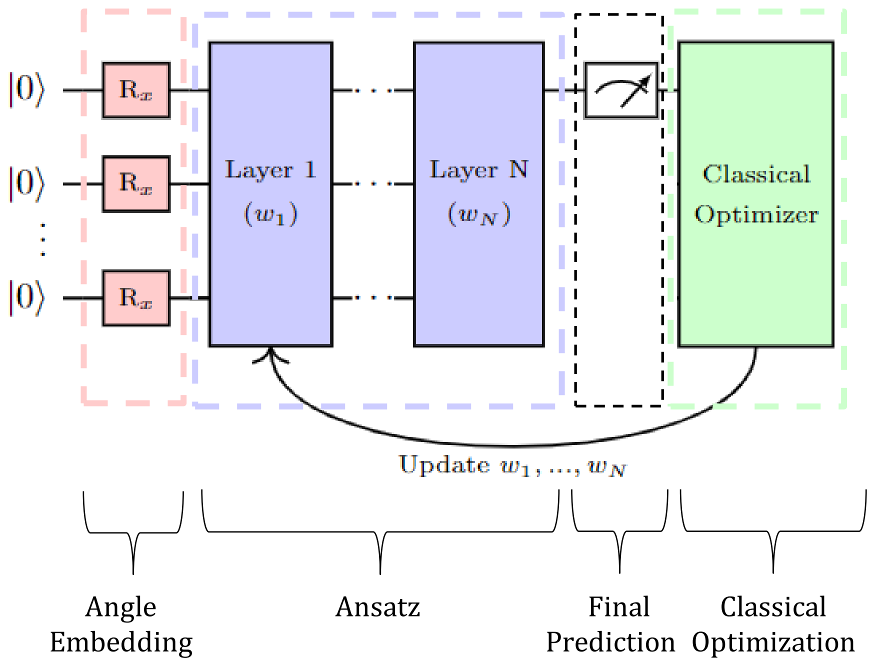
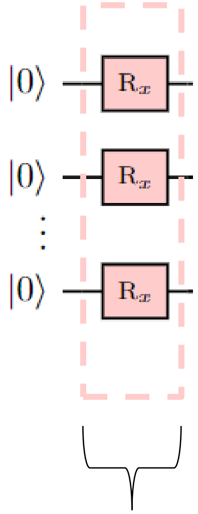


Fig 1: Variational Quantum Classifier (VQC) structure

DATA EMBEDDING



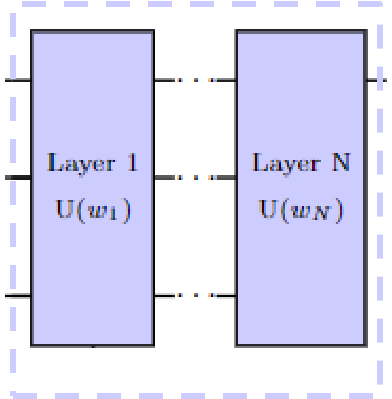
Angle Embedding

Data Embedding → Consists of encoding the classical data into a quantum state $|\psi_x\rangle$.

Angle Embedding → Each feature is encoded as an angle.

No of qubits → Corresponds to the number of features.

ANSATZ



Ansatz

Ansatz → Corresponds to a parameterized quantum circuit.

U (w) → Model circuit. Is applied to the quantum state embedded with classical information resulting in the final state $|\psi'_x\rangle = U(w)\,|\psi_x\rangle$.

w → Learning model parameters.

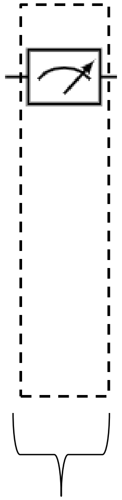
ANSATZ

Algorithm 1

Requires: $n \geq 2$, where n is the number of qubits

```
if n == 2 then
    CNOT(1, 0)
else
    for qubit ← 0 to n − 1 do
        if qubit == n − 1 then
            CNOT(qubit, 0)
        else
            CNOT(qubit, qubit + 1)
        end if
    end for
end if
```

FINAL PREDICTION



Final Prediction

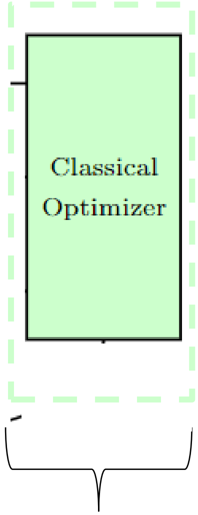
Final prediction → An **observable measurement** is performed on one of the qubits in the final state, which provides the model's prediction for the binary classification task.

Global Measuremt → With **global measuments** the gradient of the cost function **exponentially diminishes** as the **system size increase.** [1]

Local Measuremt → Employing **local observables** leads to, at worst, a **polynomially** vanishing gradient. [2]

[1] Z. Holmes, K. Sharma, M. Cerezo, P.J. Coles, PRX Quantum 3, 010313 (2022)
[2] M. Cerezo, A. Sone, T. Volkoff, L. Cincio, P.J. Coles, Nature communications 12, 1791 (2021)

CLASSICAL OPTIMIZATION



Classical
Optimization

Classical optimization → Corresponds to the use of a classical optimizer to **identify the optimal *w*.**

Cost Function → Serves as a **quantitative measure** of the **discrepancy between** the **output** state generated by the **VQC and** the **desired** target **state**.

VQC: EXAMPLE

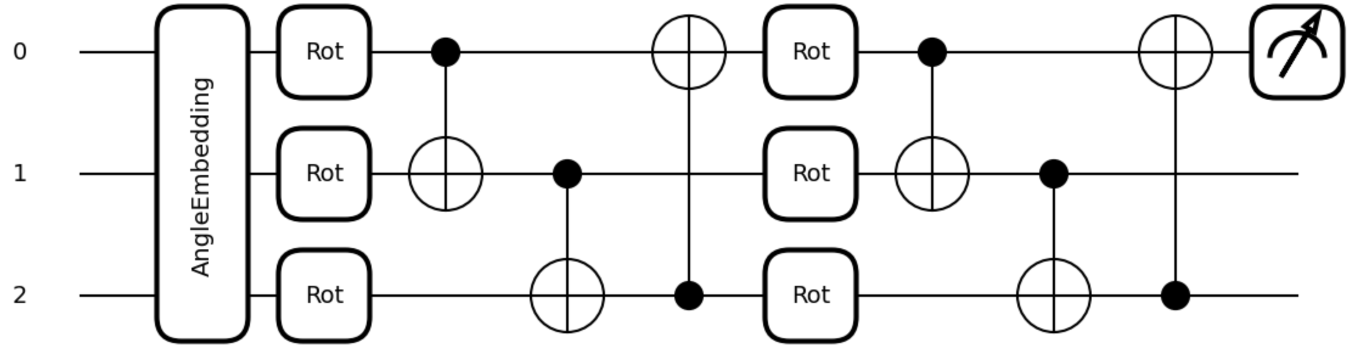


Fig 2: An example circuit for the VQC architecture used. It is comprised of 2 layers and 3 features.

IMPLEMENTATION DETAILS

Algorithm 2

```
params ← params_initialization()
for epoch ← 1 to max_epochs do
    loss ← cost(params)
    params ← optimizer.step()
    if epoch_number%5 == 0 or epoch_number
    == max_epochs then
        validation_step()
    end if
    if early_stopping_cond and epoch_number >
    min_epochs then
            break
    end if
end for
```

1 The training commences by initializing the weight vector randomly.

2 It undergoes multiple training iterations until reaching the maximum specified epochs or until the validation AUC score stabilizes.

IMPLEMENTATION DETAILS

Algorithm 2

```
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    end if
    if early_stopping_cond and epoch_number >
    min_epochs then
        break
    end if
end for
```

3

The condition for stability was defined as not achieving a superior AUC score in 20 epochs.

4

In each iteration, the model is applied to the training dataset, computing the cost function, and then updating the model parameters using the Adam optimizer.

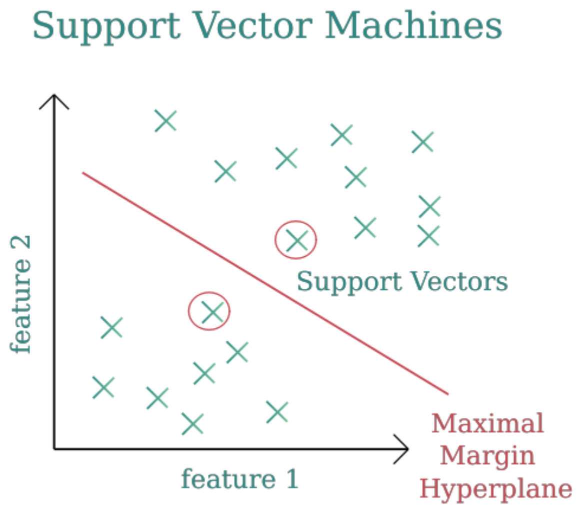
CHARACTERISTICS OF THE SIMULATION

The quantum machine learning experiments were simulated in **PennyLane**.

The quantum model's performance was evaluated on a **real quantum computer** using **PennyLane's integration with** IBM's quantum computing framework **Qiskit**.

SUPORT VECTOR MACHINE

SUPORT VECTOR MACHINES (SVM)



Why SVM? → Ensures a fair comparison.

SVM → Is trained to separate two classes of data in the feature hyperspace by **finding the hyperplane** that best separates them.

FEATURE SELECTION

FEATURE SELECTION

47 features

47 qubits

The quantum computer used only has **5 qubits**

It is necessary to **select** the 5 **best features**

Study feature selection methods

SEQUENTIAL FEATURE SELECTION (SFS)

Feature	AUC Score
$\not{E}_t$	0.817
large R-jet τ_1	0.576
large R-jet τ_3	0.316
$\mathrm{Jet}_2\ \mathrm{p_t}$	0.313
$\mathrm{Jet}_1\ \mathrm{p_t}$	0.292

Table 1: Features selected by the SBS Algorithm and their respective AUC Score on the training dataset.

Objective → Identify the most relevant features.

Description → **Initiates** with the **complete feature set** and **iteratively removes one** feature **at a time** based one their AUC score.

PRINCIPAL COMPONENT ANALYSIS (PCA)

Component	AUC Score
Component 1	0.775146
Component 3	0.715941
Component 0	0.687727
Component 14	0.630145
Component 36	0.605685

Table 2: Features selected by the SBS Algorithm and their respective AUC Score on the training dataset.

Objective → **Eliminate** feature **correlations** while preserving the original data's dimensionality.

FINDING THE OPTIMAL MODELS

GRIDSEARCH: SVM

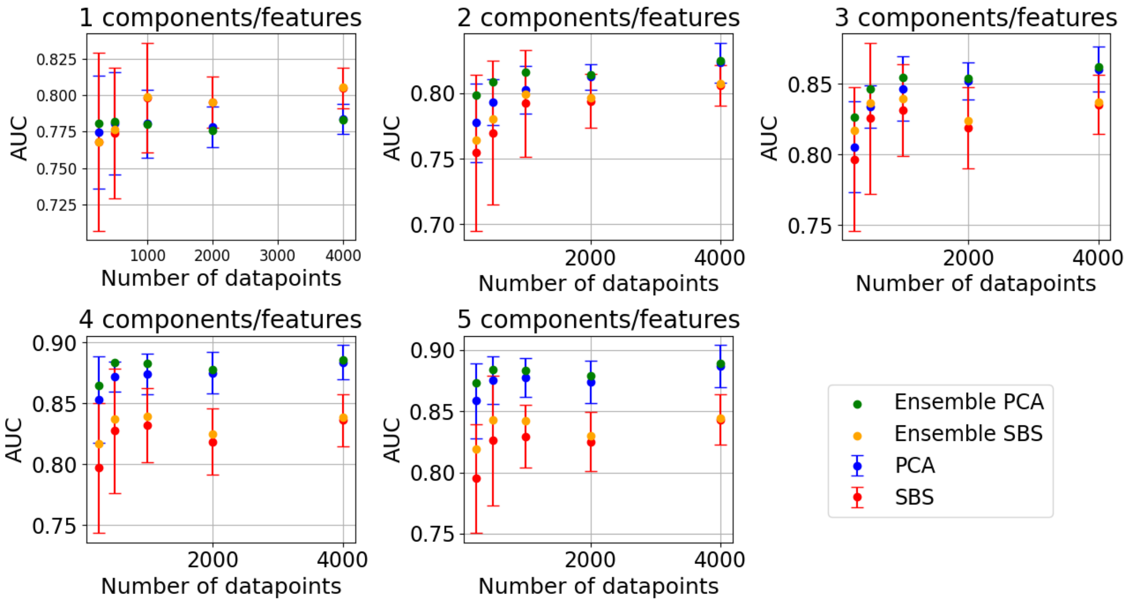
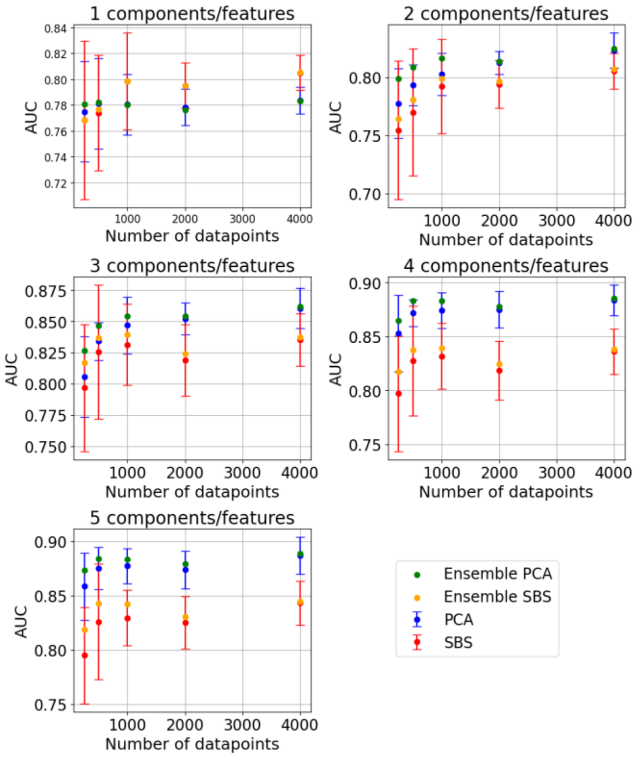


Fig 3: Plot grid representing the results for the SVM grid search. Each data point represents the AUC score on the test dataset of a different set of HP.

GRIDSEARCH: SVM



The performance achieved with 3, 4, and 5 components/features **is compatible**.

The **highest AUC** score is attained with **PCA** for **5 components** and **4000 datapoints.**

In general, PCA outperforms SBS.

PCA generates more stable results.

GRIDSEARCH:VQC

The VQC grid search is still running and therefore it is not possible to present the results yet.

REAL COMPUTER

REAL COMPUTER RESULTS (IBMQ_BELEM)

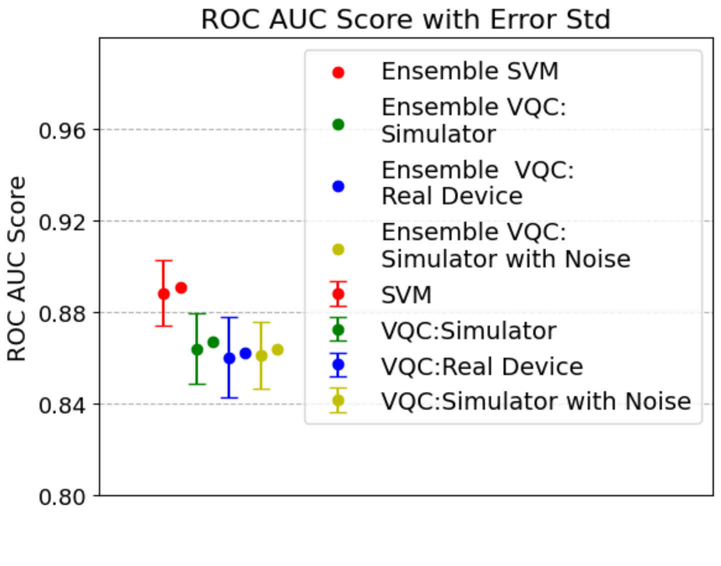


Fig 4: Comparison of the performance achieved with SVM, VQC in simulation, VQC in a real device (ibmq_belem), and VQC in simulation with quantum noise from ibmq_belem .

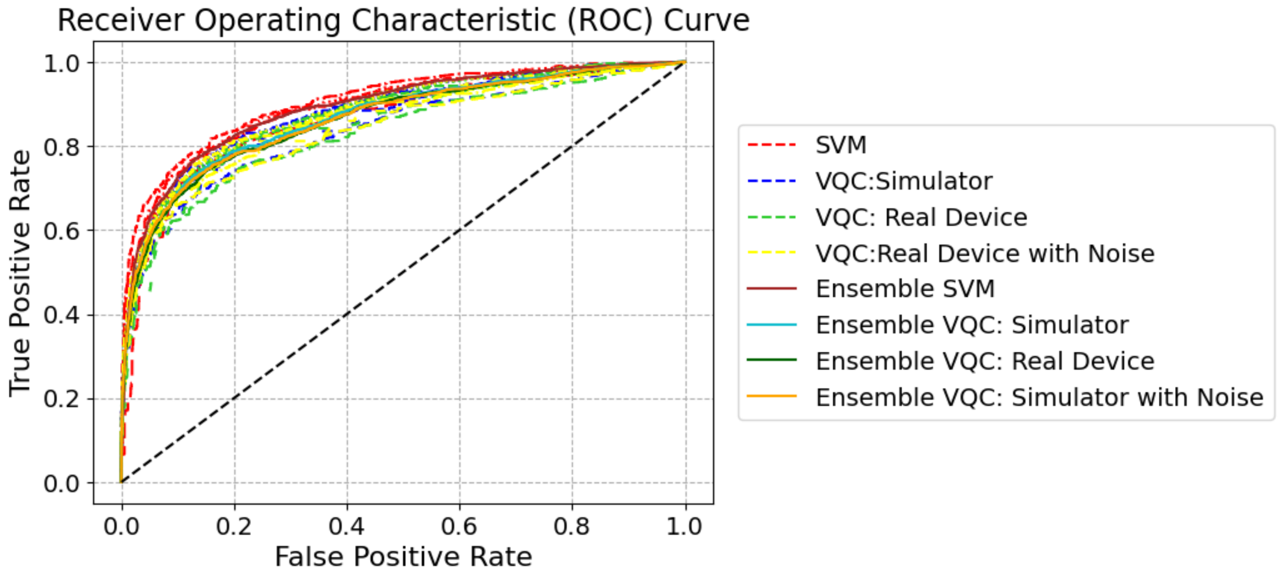
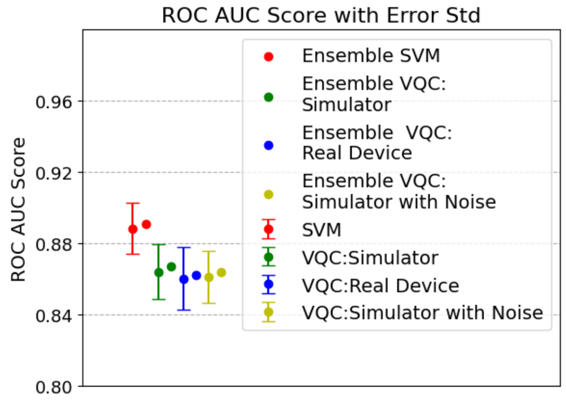
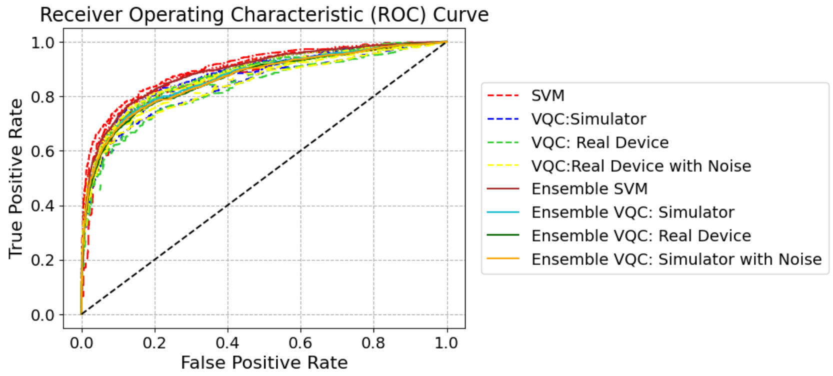


Fig 5: Variability of the ROC curve obtained for the SVM, VQC in simulation, VQC in a real device (ibmq_belem), and VQC in simulation with quantum noise from ibmq_belem.

REAL COMPUTER RESULTS





SVM and VQC results are **compatible.**

The **ensemble** method results are, in general, slightly **better than** the **mean of the** results of the **5 samples**.

Regarding the **VQC**, **simulation** and **real device** results are **compatible**.

CONCLUSION

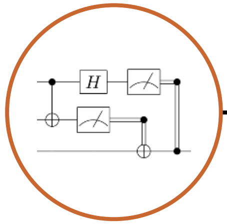
The primary **purpose** of this study is to **explore** the utilization of **QML** on **datasets** pertaining to **HEP**.

Initially, a **grid search** was conducted to identify the optimal models, which encompassed the consideration of two **feature selection techniques**: SBS and PCA.

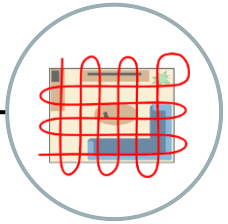
The findings relative to the **SVM grid search** indicate that **PCA**, yields superior and more stable results.

Then, a quantum model was tested in a **real quantum computer**, and it was found that the simulated, real device and SVM results are **compatible**.

FUTURE WORK



Exploring other **architectures** for the VQC to enhance its overall performance.



A comprehensive grid search encompassing SVM-specific parameters and learning rates for the VQC should be conducted, considering the **entire set of features and datapoints**.

THE END