

Optimizing Hyperparameters for Quantum Data Re-Uploaders in Calorimetric Particle Identification

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We present an application of a single-qubit Quantum Re-uploading Unit (QRU) model for particle classification tasks in calorimetric experiments, making it highly suitable for current quantum hardware constraints. Evaluated on a novel particle physics dataset, we demonstrate robust classification accuracy in a realistic use case scenario rather than relying on generic benchmarks. We explored hyperparameters tuning analysis and through global optimization methods, we identify significant hyperparameter correlations, enhancing the understanding of their interdependencies and relative importance. Furthermore, our mathematical analysis establishes that the QRU is more expressive than widely-used QML methods such as Variational Quantum Circuit (VQC). These insights show the QRU as a superior choice for practical quantum machine learning tasks.

Keywords: Quantum machine learning, Quantum re-uploading, Hyperparameter optimization, Particle classification, Fourier analysis, Expressivity, Calorimetry.

1 Introduction

The potential of quantum machine learning (QML) Biamonte et al. [2017] to resolve challenging issues in a variety of fields, including particle physics Hitran and Ellynn [2023], Team [2023], has attracted a lot of attention. The main concept of QML is to use the properties of quantum mechanics to perform multiple calculations at once, which could result in quicker classification, regression, or clustering tasks Zhou [2021], Steane [1998]. In terms of quantum

computing Preskill [2018], we are still in the Noisy Intermediate-Scale Quantum (NISQ) era Bharti et al. [2022], characterized by limited qubit counts and shallow circuit depths, posing substantial challenges for QML applications dealing with high-dimensional and nonlinear data.

Under these restrictions, the Data Re-Uploading (QRU) model, introduced by Pérez-Salinas et al. [2019], can become an attractive proposition. With the QRU model, data is encoded iteratively as rotation parameters over single-qubit circuits. This is leading to improved expressibility of the model while keeping its qubit requirements low. The QRU structure alternates data-encoding gates and trainable parameterized gates, It could be mathematically represented as:

$$U(\theta, x) = \prod_{j=1}^M e^{ig_j x} W_j e^{iV_j \theta_j}, \quad (1)$$

where x represents the classical data to be encoded, g_j and V_j are traceless Hermitian operators defining the data encoding and trainable gates, respectively and W_j are fixed unitary transformations. Unlike quantum neural networks Ezhov and Ventura [2000] and kernel quantum methods Schuld [2021], the QRU has the universal approximation property (i.e., density of approximation with incrementally encoded data), allowing it to represent complex nonlinearities that are important Glendinning [2005].

Here, we implement and assess a single-qubit QRU for a classification task that makes use of a new simulated dataset-useful in high-energy particle studies. This dataset, never used previously in the literature, contains different classes (electrons, muons and pions) making it ideal to

serve as a benchmark for multi-class classification problems that are useful for evaluating QRU performance. The datasets of high-energy particles is chosen in accordance to the recent effort towards classification and prediction of energy with QML, especially for high-dimensional datasets like LHC Team [2021], Hitran and Ellynn [2023]. We investigate the performance of the model on this dataset, reporting classification accuracy, loss and simulation environment execution time.

An integral part of our work is the systematic search and tuning of QRU hyperparameters (circuit depth, learning rate, batch size, etc.). Due to the error sensitivity of NISQ devices, there is a direct correlation between each hyperparameter and the accuracy and stability of the model Kingma [2014]. We investigate both empirical tuning to enhance model efficiency as well as preliminary tests of global optimization methods.

The main contribution of this study is a thorough analysis of the QRU performance, particularly suited to the NISQ era due to its single-qubit design. We evaluate this architecture on a previously unpublished dataset, applying it to a realistic use case rather than a generic dataset and report strong performance results for such a compact quantum circuit. Our extensive investigation into the hyperparameters of both the quantum model and training procedure elucidates their interdependencies and ranks their relative impact, allowing practitioners to finely tune the QRU according to specific criteria.

Additionally, our mathematical analysis establishes that the QRU is inherently more expressive than the widely-used Variational Quantum Circuit (VQC) Cerezo et al. [2021], highlighting VQC’s limitations not only due to qubit requirements and noisy entanglement gates but also in term of Fourier frequency boundary, thereby justifying our preference for QRU in this research.

2 Theory

To understand the reason why we chose QRU over others QML algorithms, we compare the expressive capabilities of two quantum architectures with the same number of trainable parameters θ :

- A VQC with $n = 3$ qubits and L variational layers, each composed of CNOT gates and

single-qubit Euler rotations. A single data encoding layer applies $RY(x_j)$ gates once to each qubit.

- A QRU with $n = 1$ qubit and L repeated data/parameter blocks. Each block applies the following rotation sequence for each input dimension x_j :

$$RX(\theta_0) RY(\theta_1 \cdot x_j) RZ(\theta_2)$$

This is totaling $9L$ trainable parameters in both models.

Lemma. *Let each coordinate x_j be encoded K_j times through single-parameter rotations of the form $RY(\theta_{k,j} \cdot x_j)$, where $\theta_{k,j} \in \mathbb{R}$ is a trainable parameter. Then the Fourier expansion of the output of the circuit $f(\mathbf{x})$ contains only terms:*

$$f(\mathbf{x}) = \sum_{\mathbf{n} \in \mathcal{F}} c_{\mathbf{n}} e^{i(n_1 x_1 + \dots + n_d x_d)}, \quad (2)$$

with $\mathcal{F} \subseteq \mathbb{Z}^d$ and

$$n_j \in \text{Span}_{\mathbb{Z}}\{\theta_{1,j}, \dots, \theta_{K_j,j}\} \quad (3)$$

$$\Rightarrow |n_j| \leq \sum_{k=1}^{K_j} |\theta_{k,j}|. \quad (4)$$

Implication. The Fourier support \mathcal{F} of a QRU grows linearly with the number of re-uploads L , while that of a VQC remains bounded by the single encoding layer: $K_j = 1$ for all j .

For example, with $d = 1$ and $L = 4$, we have:

$$\mathcal{F}_{\text{VQC}} \subseteq \{-1, 0, 1\}, \quad (5)$$

$$\mathcal{F}_{\text{QRU}} \subseteq \{-4, -3, \dots, 3, 4\}. \quad (6)$$

This means that the QRU can, in principle, express functions with higher-frequency components than any mono-encoding VQC, regardless of the number of qubits.

Figure 1 confirms the lemma visually: the QRU accesses a wider harmonic spectrum, providing a strictly larger function class than the VQC. This justifies the use of QRUs in applications where high-frequency resolution or functional flexibility is needed.

To corroborate the Fourier Support Lemma, we performed the following experiment for $d = 3$,

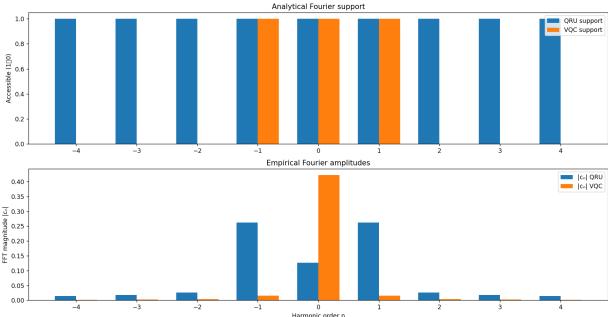


Figure 1: Comparison of analytical Fourier support (top) and empirical Fourier amplitudes (bottom) for QRU (blue) and VQC (orange). Both models use $9L$ trainable parameters.

$L = 6$, $M = 100$ and $N = 96$ points on the diagonal $\mathbf{x} = (u, u, u)$ with $u \in [-1, 1]$:

$$p_n = \frac{1}{M} \sum_{k=1}^M \mathbf{1}(|c_n^{(k)}| > \varepsilon), \quad (7)$$

$$c_n^{(k)} = \frac{1}{N} \sum_{t=0}^{N-1} f(x_t; \theta^{(k)}) e^{-i2\pi nt/N}, \quad (8)$$

where $\theta^{(k)}$ is the k -th random draw of trainable parameters and $\varepsilon = 0.05$. The resulting activation probabilities

$$\begin{aligned} p_n^{\text{QRU}} &\approx [0.86, 1.00, 0.99, 0.92, 0.70, \\ &\quad 0.34, 0.13, 0.02, 0.00, 0.00], \\ p_n^{\text{VQC}} &\approx [0.83, 0.81, 0.19, 0.04, 0.00, \\ &\quad 0.00, 0.00, 0.00, 0.00, 0.00]. \end{aligned}$$

The QRU empirically activates all harmonics up to order L , whereas the mono-encoded VQC occasionally fails to activate higher-order terms, in perfect agreement with the lemma and the analytical spectra of Figure 1.

3 Methodology

This section details the datasets, model configuration and experimental setup for evaluating QRU on a quantum simulator. We describe the data sources, baseline setups and computational environment we used in our study.

3.1 Dataset

The data used in this study are extracted from the OGCID/D2 simulation dataset [Becheva et al. \[2024\]](#). It is a set of single particle interaction

with a simplified highgranularity calorimeter inspired by CMS/HGCal [Collaboration \[2017\]](#).

This detector architecture features two main sections: the electromagnetic calorimeter (ECAL) and the hadronic calorimeter (HCAL), optimized for detecting particles of varying energies. The ECAL comprises 26 layers of lead absorbers (6.05 mm thick), while the HCAL has 24 layers of stainless steel absorbers, with 12 layers of 45 mm thickness and 12 of 80 mm, providing high resolution in capturing energy deposits. Active silicon layers are placed between absorbers, segmented into hexagonal cells with a thickness of 0.32 mm and a transverse area of approximately 1 cm² for ECAL and 4 cm² for HCAL [Team \[2023\]](#).

The D2 dataset is a collection of simulated interactions between this detector and four types of particles (muon, positive pions, electrons and photons [Team \[2021\]](#), [Hitran and Ellynn \[2023\]](#)) at different energies and with a flat incidence angle (aligned with the longitudinal detector axis). The dataset includes detailed informations on each particle event, namely the energy measurement in each cell but also extracted variaies of interest describing the geometry and the energy repartition of the hits.

For this study, only one file of electrons, pions and muons has been used `*_E10 - 100_theta0` and specifically some variables of interest known for their iscriminating power : the total energy deposited in the ECAL, the length of the particle interaction shower and the standard deviation of the energy deposits in the HCAL.

3.1.1 Execution environment

Experiments were run on a cloud server with both CPU and GPU resources, utilizing the `default.qubit` simulator and testing PennyLane Lightning for potential GPU acceleration. Although smaller circuits showed a 2.5x speedup on GPU, no significant gains were observed for larger circuits, likely due to shared cloud resources.

4 Results

This section presents the performance results of the QRU model on the particle classification task.

We first analyze the impact of individual hyperparameters, organized into model-related and training-related parameters. Then, we explore the effects of global optimization techniques, including Bayesian optimization and initial tests using Hyperband and investigate correlations between key hyperparameters.

4.1 Impact of individual hyperparameters

This subsection examines the effect of model-related hyperparameters, specifically circuit depth, input normalization, rotation gates and the number of trainable parameters per input on the classification accuracy and computational efficiency of the QRU model.

In order to assess the variability of the QRU model, we analyzed the test accuracy and loss across 50 independent runs. For each run, we reshuffled the dataset and randomly initialized the parameters θ following a Gaussian distribution centered around 0.5. The plots below illustrate the test accuracy and loss for these runs:

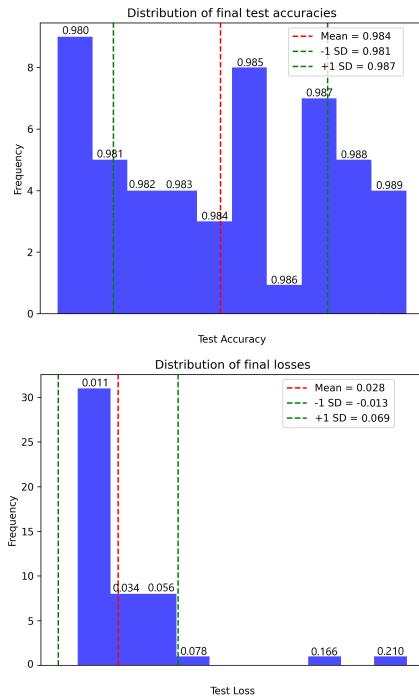


Figure 2: Left: Final test accuracy; right: Final loss over 50 runs

For the test accuracy, the mean is 0.98 with a variability of 0.002881, indicating that the results are highly consistent and centered around this value. On the test losses side, the mean is

0.028 with a variability of 0.041.

Having established the variability in the QRU's performance for classification task, we now move on to analyze how the model behaves when adjusting the depth of the quantum circuit, a critical hyperparameter for model expressivity and learning capacity.

4.1.1 Model hyperparameters

3.1.1.1 Circuit depth

The depth of the circuit represents the number of times the data is re-uploaded into the quantum circuit. It's important to note that a depth of 1 represents a quantum circuit that has not re-uploaded the input and that means it's not technically a QRU.

Figure 3 shows the evolution of the loss over 30 epochs for different values of depth. We observe a significant decrease in the loss as the depth is increasing, particularly between depths 1 and 3, where the loss drops from 0.25 to less than 0.05. Beyond a depth of 4, the loss stabilizes around 0.03, indicating that increasing the depth beyond this threshold does not significantly improve the model's performance in terms of loss minimization.

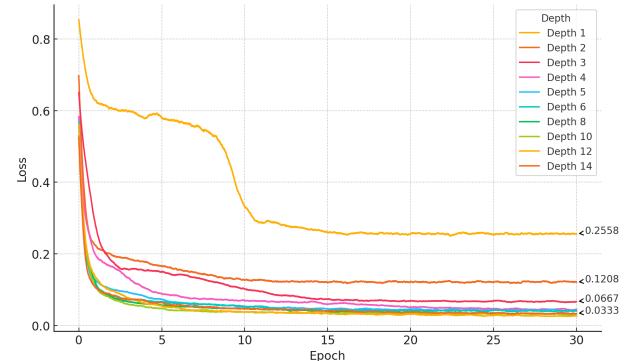


Figure 3: Evolution of the loss over epochs for different circuit depths.

Next, Figure 4 shows the evolution of test accuracy over epochs for different depth values. Similarly, we observe a rapid improvement in accuracy with shallow depths (from depth 1 to depth 3), with accuracy approaching 0.98 from a depth of 4 onwards. Again, higher depths yield only marginal gains in accuracy.

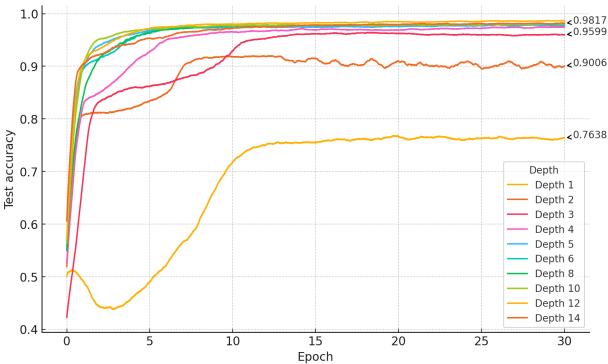


Figure 4: Evolution of test accuracy over epochs for different circuit depths.

The following three graphs (Figure 5) respectively present the execution time, final loss and final accuracy as a function of the circuit depth.

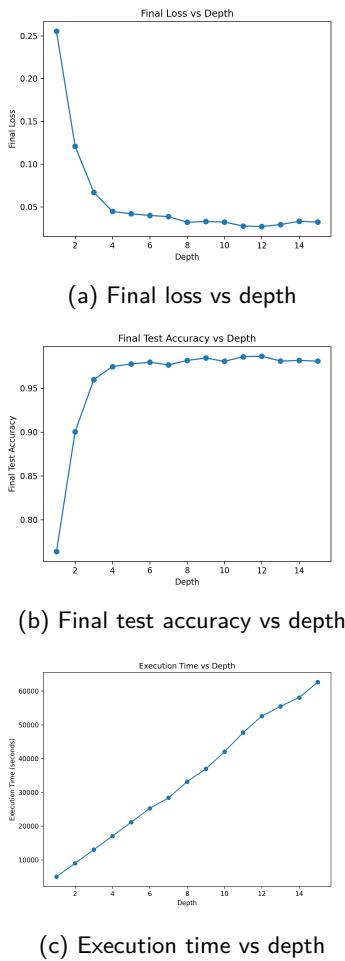


Figure 5: Comparison of execution time, final loss and final accuracy as a function of circuit depth

We observe an increase near linear in execution time with the depth (Figure 5c), with the time exceeding 60,000 seconds for a depth of 14, which is approximately 16 hours. In terms of

final loss (Figure 5a), the results show a marked improvement between depths 1 and 4, followed by stabilization from depth 5 onwards. Then, the final test accuracy (Figure 5b) follows a similar trend, plateauing around a depth of 4 with a final accuracy close to 0.98.

These results show that while increasing the circuit depth beyond 4 yields only marginal performance improvements, it comes at a significant cost in execution time. Therefore, it is essential to find a balance between circuit depth and computational efficiency for practical applications.

These results are consistent with similar findings discussed in the literature like the work 'Data Re-uploading for a Universal Quantum Classifier' Pérez-Salinas et al. [2019]. The authors show that increasing the number of re-uploading layers often boosts the expressivity of the quantum model. A caveat is that this argument is powerful as it precisely shows that expressivity is not directly proportional to the dimension of the Hilbert space and the depth of the reuploading layers. Rather, expressivity is a function of several things such as depth of the circuit, gate structure and the power of parameter tuning to exploit non-linear transformations introduced by data re-uploading:

$$\text{Expressivity} \sim g(L) \cdot h(U(\phi, \mathbf{x}), \theta), \quad (9)$$

where $g(L)$ is a non-linear function that accounts for the diminishing returns of the increasing number of layers we re-upload L , $U(\phi, \mathbf{x})$ is the parameterized unitary gates encoding the data and θ represents the tunable parameters of the circuit. Here $\dim(\mathcal{H}) = 2$ as it is for a single qubit and the expressibility is dominated primarily by the competition between the number of re-uploaded layers L and the gate structure.

As seen in our experiments, while the performance improves significantly for depths up to 4, further increases in depth provide only marginal gains. This can be explained by the bias-variance tradeoff Briscoe and Feldman [2011]: as we increase the depth, the model gains expressivity and reduces bias, but the improvements become smaller. This is likely because our classification problem is relatively simple and the additional complexity introduced by deeper circuits does not translate into significant perfor-

mance improvements. The expressivity gained from re-uploading becomes less impactful once the model complexity exceeds the requirements of the task. Therefore, there is a practical upper bound to the benefits of increasing depth in this case.

Having examined the impact of circuit depth on the QRU’s performance, we now turn our attention to the effect of the input normalization.

3.1.1.2 Input normalization

In this section, we analyze the effect of input normalization on the performance of the QRU model. Specifically, we compare two normalization ranges: 0 to 2π and $-\pi$ to π . The results are presented in terms of final loss, final test accuracy and trainability.

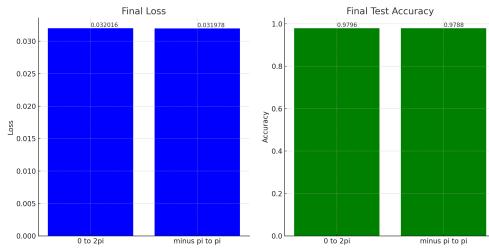


Figure 6: Comparison of final loss and final test accuracy for input normalization ranges 0 to 2π and $-\pi$ to π

As shown in Figure 6, there is no significant difference in performance between the two normalization ranges. The final mean loss is 0.032016 for 0 to 2π and 0.031978 for $-\pi$ to π , indicating virtually identical outcomes. Similarly, the final test accuracy is 0.9796 for 0 to 2π and 0.9788 for $-\pi$ to π , again showing no meaningful discrepancy.

The lack of a significant difference can be attributed to the fact that our quantum circuits γ , which govern the behavior of the QRU, are symmetric functions of the input over a period of 2π . This symmetry is highlighted in the circuit fits shown in Figure 7, where we observe similar patterns in the behavior of the circuit for 9 different configurations of θ over both normalization intervals.

Hypothesis functions [Barthe and Pérez-Salinas, 2023] generated by QRU models are de-

fined as the expectation value of a measurement observable Z applied to the output quantum state of the circuit. Mathematically, they are given by:

$$h_\theta(x) = \langle 0 | U^\dagger(\theta, x) Z U(\theta, x) | 0 \rangle, \quad (10)$$

where $U(\theta, x)$ is the parameterized quantum circuit that incorporates data encoding through iterative layers of single-qubit rotations. These hypothesis functions can be further expressed as generalized trigonometric polynomials:

$$h_\theta(x) = \sum_{\omega \in \Omega} a_\omega(\theta) e^{i\omega x}, \quad (11)$$

where Ω is the set of available frequencies determined by the data encoding scheme and $a_\omega(\theta)$ are Fourier coefficients dependent on the trainable parameters θ .

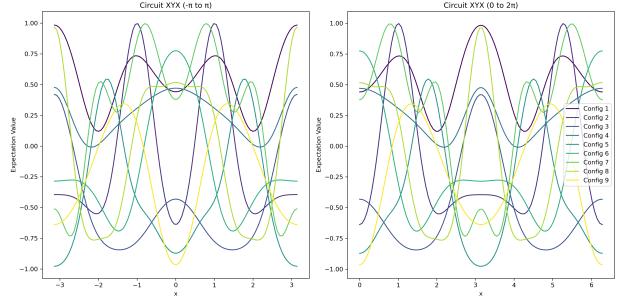


Figure 7: Hypothesis functions $h_\theta(x)$ for 9 configurations of θ for the circuit $R_x - R_y - R_x$ over the intervals $-\pi$ to π (left) and 0 to 2π (right) with a depth of 10

This graph shows that shifting the normalization range by π to the right results in fit functions that remain even functions, exhibiting similar behavior to those normalized to the left of π . As such, the expressivity does not change, which explains the lack of noticeable differences between the two ranges.

Previously, we tested the QRU model on non-normalized data and the model failed to learn properly. It could be attributed to the fact that the non-normalized values, particularly for features 2 and 3, are extremely small, as seen in Figure 8.

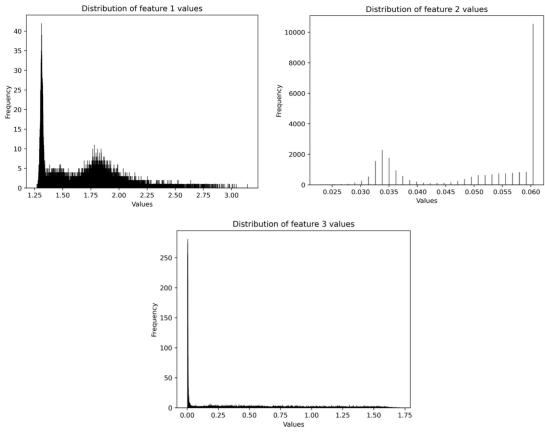


Figure 8: Feature distributions

This can be explained by considering the quantum state of the qubit: when the input values are very small, the qubit undergoes minimal rotations on the Bloch sphere, making it difficult to differentiate between states when the quantum measurement is performed along the Z-axis.

3.1.1.3 Rotation gates

In this experiment, we analyzed the impact of different types of quantum rotations on the performance of the QRU model. We compared six circuits based on successive rotations of types R_x , R_y and R_z , with the following structure:

$$\begin{aligned}
 R_x - R_y - R_x : |q\rangle & \xrightarrow{\boxed{R_X(\theta_i)}} \boxed{R_Y(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_X(\theta_{i+2})}} \text{Measure} & c \\
 R_x - R_z - R_x : |q\rangle & \xrightarrow{\boxed{R_X(\theta_i)}} \boxed{R_Z(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_X(\theta_{i+2})}} \text{Measure} & c \\
 R_y - R_x - R_y : |q\rangle & \xrightarrow{\boxed{R_Y(\theta_i)}} \boxed{R_X(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_Y(\theta_{i+2})}} \text{Measure} & c \\
 R_y - R_z - R_y : |q\rangle & \xrightarrow{\boxed{R_Y(\theta_i)}} \boxed{R_Z(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_Y(\theta_{i+2})}} \text{Measure} & c \\
 R_z - R_x - R_z : |q\rangle & \xrightarrow{\boxed{R_Z(\theta_i)}} \boxed{R_X(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_Z(\theta_{i+2})}} \text{Measure} & c \\
 R_z - R_y - R_z : |q\rangle & \xrightarrow{\boxed{R_Z(\theta_i)}} \boxed{R_Y(\theta_{i+1} \times x_j)} \xrightarrow{\boxed{R_Z(\theta_{i+2})}} \text{Measure} & c
 \end{aligned}$$

The performance of each type of circuit was evaluated in terms of final loss and final test accuracy. Figure 9 below illustrates the results obtained for these metrics.

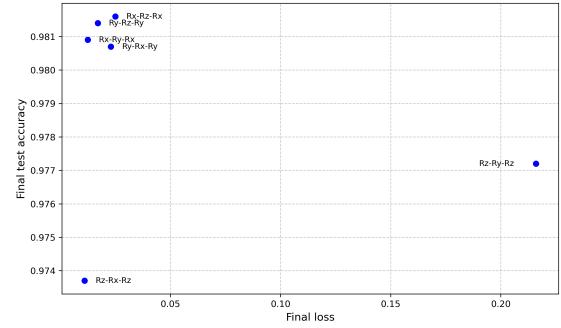


Figure 9: Performance of different circuits based on rotation types

The results show that the $R_x - R_y - R_x$ circuit achieves the best performance in terms of final loss, indicating that this combination of rotations allows for better optimization of the model. On the other hand, the $R_z - R_y - R_z$ circuit has the lowest final test accuracy, significantly lower than the other circuits. Conversely, the $R_x - R_z - R_x$ circuit and the $R_y - R_x - R_y$ circuit achieve high accuracy, with relatively low loss, showing that these rotation configurations offer a good balance between accuracy and stability. However, the $R_y - R_z - R_y$ circuit shows a higher final loss, suggesting that this type of rotation may introduce larger fluctuations in parameter optimization. Overall, the results indicate that rotations involving only R_x and R_y are more stable and perform better than those involving R_z .

Hubregtsen et al. (2021) Hubregtsen et al. [2021] explored the correlation between the capacity of parameterized quantum circuits (PQC) to explore the Hilbert space and classification accuracy. They define a measure of expressibility, which quantifies the ability of a PQC to uniformly explore the Hilbert space, through the Kullback-Leibler divergence (DKL) between the fidelity distribution of the quantum states generated by the PQC and that of random Haar states. The expressibility is given by the following equation:

$$\text{Expr} = D_{\text{KL}}(P_{\text{PQC}}(F; \Theta) || P_{\text{Haar}}(F)), \quad (12)$$

where P_{PQC} is the fidelity distribution of the PQC and P_{Haar} is that of the random Haar states. The article concludes that rotations R_X , R_Y and R_Z should be used together to maximize expressibility and therefore accuracy. None of these rotations is intrinsically superior, but their combina-

tion allows full exploration of the Hilbert space. This is directly related to the following theorem:

Theorem 1 (Euler's theorem on rotations)

In a three-dimensional space, any rotation can be represented by a combination of elementary rotations around the x , y and z axes, respectively denoted as R_x , R_y and R_z . More precisely, any rotation can be expressed as a single rotation by an angle θ around a fixed axis, according to the following decomposition:

$$R(\theta, \hat{n}) = R_z(\phi)R_y(\theta)R_x(\psi) \quad (13)$$

where θ is the total rotation angle and \hat{n} is the unit vector describing the rotation axis.

Nevertheless, our results show that the combination of R_x and R_y gates in quantum data re-uploading circuits tends to offer better performance in terms of accuracy and loss minimization compared to R_x . This may simply arise from the fact that during a measurement, we project our quantum state onto the Z-axis and therefore, rotating around the Z-axis does not change the projection of the qubit on the Z-axis.

This pushes us to test other types of rotations, which we could call "triplets" ($R_x - R_y - R_z$), involving rotations around all three axes, rather than using simpler "sandwich" rotations like in our case. We plotted the QRU functions for the same depth and the same combination of theta parameters for a "sandwich" circuit and a "triplet" circuit and the results are presented in Figure 10.

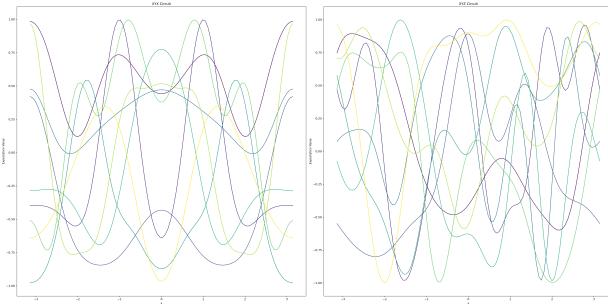


Figure 10: Hypothesis functions $h_\theta(x)$ for 9 configurations of θ for the circuit $R_x - R_y - R_x$ (left) and $R_x - R_y - R_z$ (right).

We observe that "sandwich" circuits are constrained to be even functions of the input,

whereas "triplet" circuits have more flexibility. Theoretically, this should result in better expressivity. Figure 11 shows the results obtained with $R_x - R_y - R_x$ quantum circuit.

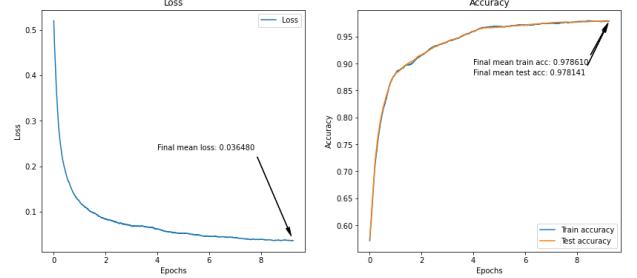


Figure 11: Performance of the "triplet" quantum circuit

The final mean loss is 0.036480, with a final mean train accuracy of 0.978610 and test accuracy of 0.978141. Comparing this with the "sandwich" circuits using only two rotations, such as $R_x - R_y - R_x$ or $R_x - R_z - R_x$, where the final accuracies were slightly higher and with lower final losses, it becomes evident that the two-rotation circuits tend to outperform in minimizing loss in our case. While three-rotation circuits like $R_x - R_y - R_z$ theoretically offer higher expressibility, in this specific case, the increased complexity does not significantly improve accuracy, but instead results in a slightly higher loss. This suggests that two-rotation circuits provide a simpler yet equally effective approach for our type of classification tasks, balancing between expressibility and optimization stability.

Next, we analyze how the number of trainable parameters per input affects the model's performance.

3.1.1.4 Number of trainable parameters per input

In this part, we analyze the impact of varying the number of parameters θ per input on the performance of the QRU model. We tested five different quantum circuit configurations, each with an increasing number of parameters per input, as described below:

1 parameter θ per input:

$$|q\rangle \boxed{R_X(\theta_i)} \boxed{R_Y(x_j)}$$

2 parameters θ per input:

$$|q\rangle \boxed{R_X(\theta_i)} \boxed{R_Y(x_j)} \boxed{R_X(\theta_{i+1})}$$

3 parameters θ per input:

$$|q\rangle [R_X(\theta_i)] [R_Y(\theta_{i+1} \times x_j)] [R_X(\theta_{i+2})]$$

4 parameters θ per input:

$$|q\rangle [R_X(\theta_i)] [R_Y(\theta_{i+1} \times x_j + \theta_{i+2})] [R_X(\theta_{i+3})]$$

5 parameters θ per input:

$$|q\rangle [R_X(\theta_i)] [R_Y(\theta_{i+1}^2 \times x_j + \theta_{i+2} \times x_j + \theta_{i+3})] [R_X(\theta_{i+4})]$$

The results of these tests are shown in Figure 12.

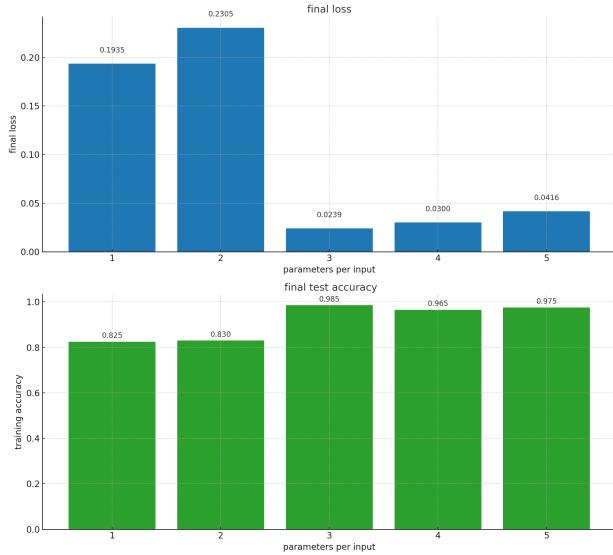


Figure 12: Performance of the QRU model based on the number of parameters per input. Top: final loss; Bottom: final test accuracy.

As seen in Figure 12, the final loss decreases dramatically when moving from 1 or 2 parameters per input (0.1935 and 0.2305, respectively) to 3 parameters, where the final loss drops to 0.0239. However, after 3 parameters per input, the final loss slightly increases again for 4 and 5 parameters (0.0300 and 0.0416, respectively). This indicates that increasing the number of parameters per input beyond 3 does not significantly improve loss minimization and may even complicate optimization.

Similarly, the final test accuracy improves from 0.825 with 1 parameter to 0.985 with 3 parameters. However, as with the loss, the accuracy plateaus and slightly decreases with 4 and 5 parameters (0.965 and 0.975). This suggests that 3 parameters per input represent the optimal configuration for balancing model complexity and performance in terms of both accuracy and loss. In summary, while optimizing the number

of parameters per input improves the expressivity and performance of the quantum circuit, it also increases the computational complexity. In the next section, we explore the use of GPU acceleration to reduce execution time of the QRU model.

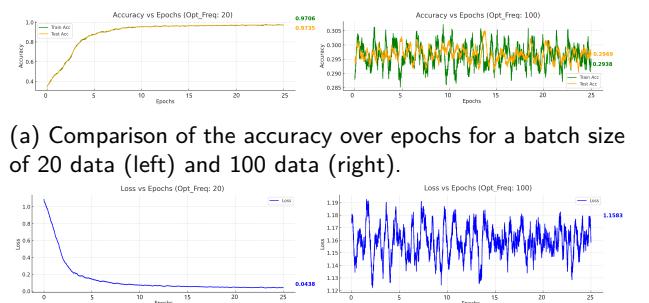
After evaluating the QRU model’s performance based on individual hyperparameter variations, we now move to a more comprehensive approach by considering the optimization of all hyperparameters simultaneously.

4.1.2 Training hyperparameters

Here, we explore the impact of training-related hyperparameters, including batch size, optimizer, loss function and learning rate, on model convergence, stability and performance.

3.1.2.1 Batch Size

The idea behind using different batch sizes is to accumulate gradients over a certain number of examples before performing an optimization step. As shown in the Figure 13a and 13b, the results vary significantly depending on the batch size. With a batch size of 20, the final test accuracy reaches 0.9735, with a final loss of 0.0438, showing stable and efficient behavior. However, when the batch size is increased to 100, the test accuracy drops dramatically to 0.2969 and the final loss rises to 1.1583, suggesting that the model struggled to learn.



(a) Comparison of the accuracy over epochs for a batch size of 20 data (left) and 100 data (right).

(b) Comparison of the test loss over epochs for a batch size of 20 data (left) and 100 data (right).

Figure 13: Comparison of the loss and accuracy over epochs for a batch size of 20 data (left) and 100 data (right).

Table 1 below summarizes the results for different batch sizes. The trainability metric, calculated as the area under the loss curve dur-

ing training, measures how easily the model can learn. It is calculated using the following equation:

$$\text{Trainability} = \int_0^E \text{Loss}(e) de \quad (14)$$

E denotes the total number of training epochs. A high trainability value indicates that the model maintains a high loss during training, which means it struggles to converge. Conversely, a lower trainability value suggests better convergence, as the loss decreases rapidly during training.

Batch size	Final train acc	Final test acc	Trainability	Execution time (s)	Final loss
1	0.9804	0.9798	0.0660	259282.30	0.0311
5	0.9780	0.9771	0.1028	256280.94	0.0354
20	0.9726	0.9729	0.1924	236998.85	0.0433
100	0.2981	0.2968	1.6949	232299.19	1.1590

Table 1: Metrics for different batch sizes

Batch size plays in quantum model training [Tüysüz et al.] and smaller batch sizes generally lead to slower convergence but achieve good final accuracy with more iterations. Larger batch sizes, on the other hand, tend to converge faster and avoid barren plateaus McClean et al. [2018], but may not always result in the best final accuracy. We can describe gradient variance with equation 15:

$$O = \frac{1}{N} \sum_{i=1}^N Z_i \otimes 1_{\bar{i}} \quad (15)$$

where Z_i is the Pauli-Z operator applied to the i -th qubit and $1_{\bar{i}}$ is the identity operator on the other qubits. This equation shows that increasing the batch size can reduce gradient variance, helping the model avoid barren plateaus and improving the stability of the training process.

We observe a slightly different result in our experiments. Notice that though smaller batch sizes still achieve the best final accuracy, larger batch sizes result in substantially worse performance both on accuracy and loss. This difference with theory can be attributed to the simplicity of our particular problem. While larger batch sizes are very appealing in more complex problems because they increase expressivity and help avoid barren plateaus, in the simple tasks we are considering here they might give rise to too high gradient variance thereby worsening learning performance. The latter takes advantage of

with-loadable batch sizes, meaning the model becomes more trainable, providing evidence that the model fails to optimize with a batch size of 100. On the other hand, larger batches or, even more, no batching (as in stochastic gradient presumably use SGD) give lower trainability and usually better performance, implying that they are ready for simple tasks where higher precision is not required. Further details on this observation will be explored in future work that will focus on understanding the reasons underlying these observations.

We now turn to the analysis of the optimizer, a key hyperparameter that influences the model’s convergence speed and overall performance.

3.1.2.2 Optimizer

We compare here the performance of different optimizers, including SGD, RMSProp and Adam, based on their impact on the performances of the QRU. Table 2 summarizes the results of the three different optimizers.

Optimizer	Execution time (s)	Final test accuracy	Final loss	Trainability
RMSprop	142569.70	0.8437	0.1086	0.1809
SGD	21217.02	0.3342	1.0244	2.9868
Adam	143880.52	0.9836	0.020732	0.7758

Table 2: Performance comparison of optimizers

SGD (Stochastic Gradient Descent) is the simplest optimizer, updating parameters using only the gradient of the loss function. It calculates the gradient for each batch and updates the parameters as follows:

$$\theta_{t+1} = \theta_t - \eta \nabla_{\theta} J(\theta_t) \quad (16)$$

where θ_t is the model parameter at step t , η is the learning rate and $J(\theta_t)$ is the loss function.

RMSProp (Root Mean Square Propagation) adapts the learning rate by dividing it by a moving average of the square of the gradients. This helps RMSProp handle problems where the magnitude of the gradients varies greatly:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{v_t + \epsilon}} \nabla_{\theta} J(\theta_t) \quad (17)$$

where v_t is the exponentially weighted moving average of the squared gradients and ϵ is a small value to prevent division by zero.

Adam (Adaptive Moment Estimation) combines ideas from both RMSProp and momentum. It calculates the exponentially weighted average of both the gradients and the squared gradients:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1)g_t \quad (18)$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)g_t^2$$

where m_t and v_t are the first and second moment estimates (similar to momentum), β_1 and β_2 are decay rates and g_t is the gradient. The parameter update is then given by:

$$\theta_{t+1} = \theta_t - \eta \frac{m_t}{\sqrt{v_t} + \epsilon} \quad (19)$$

SGD has the fastest execution time but it shows lower final test accuracy and higher trainability compared to RMSProp and Adam. This may be due to its lack of adaptive learning rates, causing slower convergence. The adaptive learning rate mechanism of RMSProp helps it converge faster than SGD but it shows worse performance in terms of accuracy and final loss compared to Adam. Adam's slightly higher execution time could be due to the additional calculations required for the first and second moment estimates.

The figure below (Figure 14) compares several optimizers derived from Adam, including Adamax, Nadam, Adagrad, Adadelta and AdamW.

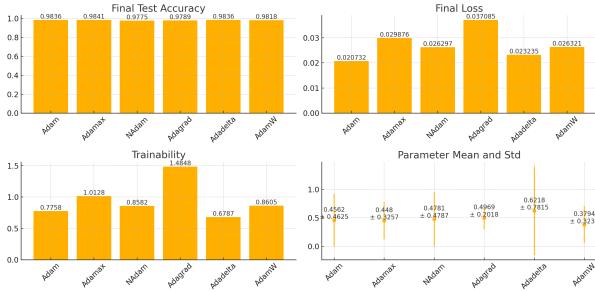


Figure 14: Comparison of Adam-derived optimizers across metrics

Each Adam variant brings slight modifications to the original algorithm. Adamax uses the infinity norm (instead of the second norm), making it more stable in certain cases. Nadam introduces Nesterov momentum into Adam, allowing for faster convergence in some settings. Adagrad adapts the learning rate based on the history

of gradients, making it suitable for sparse data but leading to slower learning in the long run. Adadelta dynamically adjusts the learning rate without needing an initial learning rate, making it more resilient to noisy data. And finally, AdamW modifies the weight decay method to achieve better generalization. As seen in the results, the performance of these optimizers is closely tied to the specific characteristics of the quantum circuit. Adagrad, for example, shows higher trainability so it suffers from slower learning, which is reflected in its higher final loss.

With the optimizer performance thoroughly analyzed, we now turn our attention to the loss function used for the training.

3.1.2.3 Loss Function

We explored three different loss functions: L1, L2 and Huber. These are used to measure the discrepancy between predicted values \hat{y} and actual values y . The L1 loss is defined as:

$$L1(y, \hat{y}) = \sum_{i=1}^n |y_i - \hat{y}_i| \quad (20)$$

It computes the sum of the absolute differences between predictions and true values, making it robust to outliers but slower to converge. The L2 loss, on the other hand, is given by:

$$L2(y, \hat{y}) = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (21)$$

This function amplifies larger errors by squaring the differences, making it more sensitive to outliers. Lastly, the Huber loss is a hybrid of L1 and L2:

$$L_\delta(y, \hat{y}) = \begin{cases} \frac{1}{2}(y - \hat{y})^2 & \text{if } |y - \hat{y}| \leq \delta \\ \delta(|y - \hat{y}| - \frac{1}{2}\delta) & \text{otherwise} \end{cases} \quad (22)$$

Huber behaves like L2 for small errors and like L1 for large errors, offering a balance between handling outliers and efficient optimization.

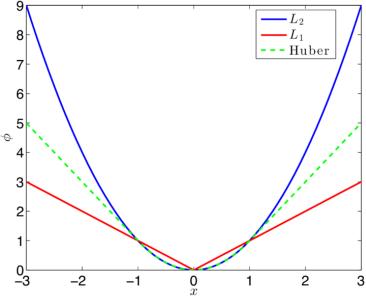


Figure 15: Difference between the three loss functions used

The results of our experiments using these loss functions over 30 epochs are shown in the figure 16. We observe that while the final loss values differ significantly between the functions, the final test accuracy remains nearly the same for all three.

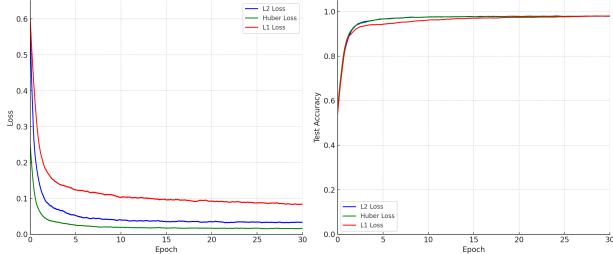


Figure 16: Evolution of the loss and the test accuracy over the epochs with the three different loss function

The difference in final loss values between the loss functions can be explained by the optimization properties of each function. For instance, the Huber loss, which combines aspects of both L1 and L2 losses, is particularly useful for handling outliers, making it less sensitive to quantum noise. This robustness allows for better minimization of the final loss.

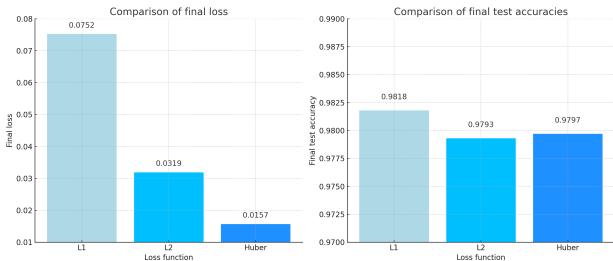


Figure 17: Comparison of the final loss and the final test accuracy with the three different loss function

While different loss functions may yield better minimization in terms of loss, they do

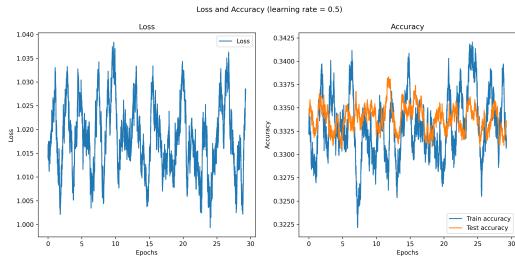
not necessarily change the decision boundaries in quantum machine learning models Aktar et al. [2024]. This explains why we observe similar test accuracy across all the loss functions despite different loss values. The stability in test accuracy is also tied to the expressibility and generalization capabilities of quantum classifiers. The decision boundaries, particularly in data re-uploading quantum classifiers, remain stable across different loss functions, provided the quantum circuit architecture is the same, as the data's separability isn't significantly affected by the choice of loss function. This explains why, despite Huber loss achieving lower final loss values, the test accuracy remains close to that of L1 and L2 losses. The choice of loss function in quantum models often optimizes gradients but does not drastically alter the classification performance.

We do not use cross-entropy as the loss function here because we have only a single qubit, meaning the outputs of our quantum circuit are a single value between -1 and 1. To use cross-entropy as the loss function, we would need a circuit with three qubits. However, this would no longer be comparable with the other tests using different loss functions, as the number of qubits also affects the results and we would lose the same reference pipeline for comparing losses. This will likely be part of future work involving multi-qubit QRUs to assess whether cross-entropy provides any advantage.

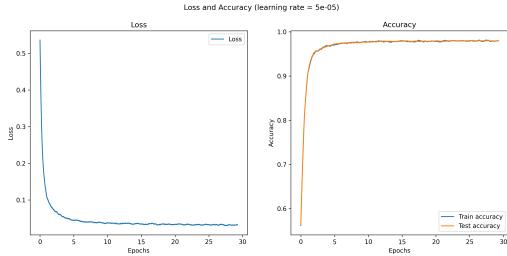
Next, we turn to the performance of the QRU when using different learning rates.

3.1.2.4 Learning Rate

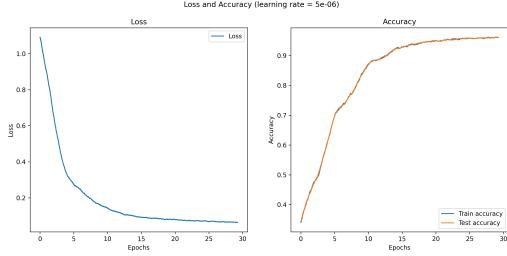
The goal of this section is to examine the impact of different initial learning rates on the model's convergence, final accuracy and loss. The results shown in Figure 18 highlight the impact of different learning rates on model performance.



(a) Learning rate = 0.5



(b) Learning rate = 5e-05

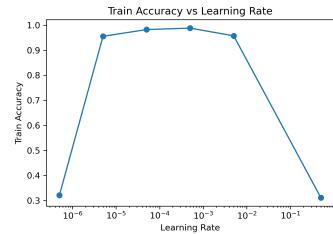


(c) Learning rate = 5e-06

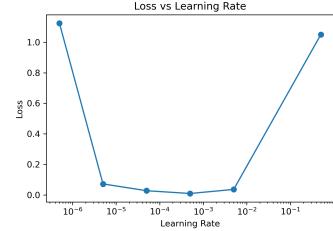
Figure 18: Loss and accuracy for different learning rates: 0.5 (18a), 5e-05 (18b) and 5e-06 (18c).

For a learning rate of 0.5 (Figure 18a), we observe significant oscillations in both loss and accuracy, indicating instability due to large updates, with accuracy remaining around 0.33. In contrast, the learning rate of 5e-05 (Figure 18b) leads to smooth convergence, with accuracy reaching near 1.0, showing a good balance between stability and learning speed. Finally, the smaller learning rate of 5e-06 (Figure 18c) provides stable learning but slower convergence, with accuracy improving more gradually. These results suggest that 5e-05 is optimal, offering a good trade-off between speed and stability.

As shown in the graphs (Figures 19a and 19b), high learning rates such as 5×10^{-1} result in higher loss and instability in the model’s performance. In contrast, moderate learning rates like 5×10^{-5} and 5×10^{-6} show better convergence, with lower final loss and higher accuracy.



(a) Evolution of accuracy as a function of lr.



(b) Evolution of loss as a function of lr.

Figure 19: Comparison of accuracy (19a) and loss (19b) as a function of lr

Table 3 presents the final loss and accuracy metrics for different learning rates:

Learning rate	$5e^{-1}$	$5e^{-3}$	$5e^{-4}$	$5e^{-5}$	$5e^{-6}$	$5e^{-7}$
Loss	1.050276	0.035826	0.009174	0.027362	0.071839	1.124110
Train accuracy	0.311538	0.957692	0.988462	0.982692	0.955769	0.321538
Test accuracy	0.323462	0.953077	0.985385	0.975385	0.960000	0.363846

Table 3: Final loss, train accuracy and test accuracy for different learning rates.

The experiments demonstrate that moderate learning rates yield the best performance. With a learning rate of 5×10^{-4} , the model reaches a test accuracy of 98.5%, outperforming both higher and lower rates. The results also show that for very small initial learning rates, there is a degradation in performance. This could be due to the fact that the model has not fully converged within the 30 epochs, or it might be trapped in a local minimum. An ongoing study is looking at whether launching the experiment with a small initial learning rate and different random seeds might yield a lower final loss compared to using higher initial learning rates.

In our experiments, we implemented an adaptive learning rate schedule to improve model convergence. The goal of this approach is to start with a relatively high learning rate, allowing the model to learn quickly at the beginning and then reduce the learning rate at specific milestones.

This reduction helps the model fine-tune its parameters as it approaches convergence, leading to more stable results.

The learning rate schedule is as follows:

1. The initial learning rate is set to 0.005.
2. At the halfway point in the total number of epochs, the learning rate is divided by 10 to slow down updates and enable more precise learning.
3. At three-quarters of the way through the epochs, the learning rate is further divided by 10 to refine the convergence even more.

Figure 20 illustrates how the learning rate decreases across epochs, using the described step-wise reduction scheme.

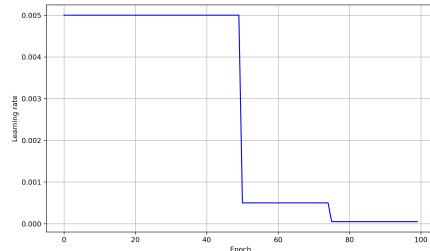


Figure 20: Adaptive learning rate schedule showing the gradual reduction in learning rate over training epochs.

However, the results show that this approach did not provide any benefit compared to letting the Adam optimizer manage the learning rate automatically.

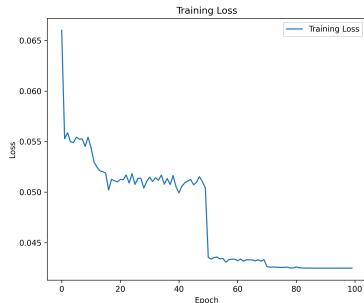


Figure 21: Evolution of the loss with adaptatif learning rate

Despite using 100 epochs to ensure convergence between each learning rate change, the results were worse than those obtained with the Adam optimizer in automatic mode.

Next, we move on to the analysis of the loss function, another key component that directly influences the model’s performance.

4.2 Global optimization

In this subsection, we discuss the application of global optimization methods to the QRU model to enhance hyperparameter tuning. We focus on Bayesian optimization as a primary method and briefly discuss our initial tests with Hyperband. We also analyze the observed correlations between key hyperparameters and their combined effects on model performance.

4.2.1 Bayesian optimization

Bayesian optimization Alaa and van der Schaar [2019] is an efficient method for hyperparameter optimization when model evaluations are expensive. The objective function $f(x)$, which we seek to optimize, is modeled using a Gaussian process (GP). The GP is defined by a mean function $\mu(x)$ and a covariance function $k(x, x')$:

$$f(x) \sim \mathcal{GP}(\mu(x), k(x, x')) \quad (23)$$

The Upper Confidence Bound (UCB) acquisition function guides the selection of the next point to evaluate by maximizing the sum of the predicted mean $\mu(x)$ and an upper confidence bound proportional to the uncertainty $\sigma(x)$:

$$UCB(x) = \mu(x) + \kappa\sigma(x) \quad (24)$$

Where κ is a parameter balancing exploration (regions where $\sigma(x)$ is high) and exploitation (regions where $\mu(x)$ is high). Once a point x_t is evaluated, the GP is updated using the newly observed data. The updated mean $\mu_{t+1}(x)$ is calculated by conditioning the GP on the previous points $X_t = \{x_1, x_2, \dots, x_t\}$ and their corresponding observations $y_t = \{f(x_1), f(x_2), \dots, f(x_t)\}$:

$$\mu_{t+1}(x) = k(x, X_t)^\top K(X_t, X_t)^{-1} y_t \quad (25)$$

Here, $K(X_t, X_t)$ is the covariance matrix of the previously evaluated points and $k(x, X_t)$ is the covariance vector between the new point x and the previously evaluated points X_t . This equation leverages the correlations between x and past points to compute the new expected mean.

The variance $\sigma_{t+1}^2(x)$ is updated similarly, representing the uncertainty of the GP's prediction at point x after conditioning on the previously observed data:

$$\sigma_{t+1}^2(x) = k(x, x) - k(x, X_t)^\top K(X_t, X_t)^{-1} k(x, X_t) \quad (26)$$

In this equation, $k(x, x)$ represents the variance at point x (before conditioning) and the second term adjusts this variance based on how correlated x is with the previously evaluated points. The result gives the updated uncertainty for x . This process is repeated until convergence, efficiently finding the optimal hyperparameters.

In our work, we have integrated Bayesian optimization into the training process to search for the best hyperparameters for our model. We defined the hyperparameter search space as follows:

- **depth:** {1, 2, 3, 4, 5, 6, 7, 8, 9, 10}
- **learning rate:** {0.5, 0.05, 0.005, 0.0005, 0.00005, 0.000005, 0.0000005}
- **loss function:** {L1, L2, Huber}
- **optimizer:** {SGD, RMSprop, Adam, Adamax, NAdam, Adagrad, Adadelta, AdamW}

The objective function takes a set of hyperparameter values, trains the model with these values and returns the average loss. We used the `gp_minimize` function from `scikit-optimize` to execute Bayesian optimization and find the best hyperparameters: `gp_minimize(objective, space, n_calls=50, random_state=0, acq_func="UCB", kappa=4)`.

Figure 22 shows the obtained results: on the left, the evolution of the final loss and on the right, the evolution of the final test accuracy as a function of different optimization runs.

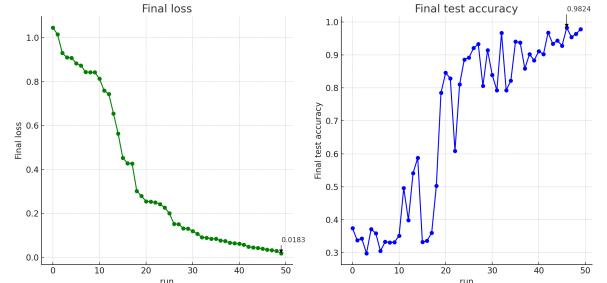


Figure 22: Evolution of the loss (left) and accuracy (right) during Bayesian optimization

The optimal configuration that resulted in the smallest final loss is: `depth=7, learning_rate=0.5, loss_function=Huber, optimizer=Adagrad` with a score of 0.018. Although this configuration minimized the loss, the final accuracy associated with this configuration remains slightly lower than that of other configurations, reaching 0.978. In fact, the best accuracy achieved was 0.9824, obtained with the configuration `depth=5, learning_rate=0.5, loss_function=L2, optimizer=Adadelta`, but this configuration produced a slightly higher loss : 0.0344.

One notable aspect of the Bayesian optimization results is the relatively high learning rate of 0.5. Such a rate might seem too large in a classical optimization context. However, the use of the Adagrad and Adadelta optimizer compensates for this effect. Adagrad dynamically adjusts the learning rate based on the accumulated gradients during training. This mechanism allows the model to converge quickly at the beginning of training by exploring promising regions of the parameter space. This could be likely why Bayesian optimization identified a configuration with a high initial learning rate as optimal.

These results show that manual optimization can also lead to highly performant configurations, notably with an accuracy slightly higher than that obtained through Bayesian optimization, reaching 0.9854 with a learning rate of $5e^{-4}$. Manual optimization thus provides a better understanding of the individual impact of each hyperparameter, while global optimization allowed us to see which combinations of hyperparameter values were correlated.

In conclusion, although global Bayesian opti-

mization effectively reduced the loss and quickly explored the hyperparameter space, manual hyperparameter optimization allowed for slightly better accuracy maximization. These results demonstrate the importance of understanding hyperparameter impact and adopting a combined approach, using both Bayesian optimization to efficiently explore hyperparameter combinations and manual optimization to fine-tune the most sensitive parameter settings.

4.2.2 Hyperband optimization

We also tested a global hyperparameter optimization method presented by Charles Moussa et al. for quantum neural networks [Moussa et al. \[2022\]](#). HyperBand stands out for its adaptive approach, allocating a computational budget to several hyperparameter configurations and progressively eliminating the less promising ones. Optimization can be further improved by integrating techniques such as fANOVA, priors and surrogates.

To analyse the importance of hyperparameters and their interaction, we decomposed the variance of a model performance using an fANOVA model (Functional Analysis of Variance). It portions out this variance for each hyperparameter where the portion corresponds to their marginal effects, i.e., average effect of a given hyperparameter on performance. Priors on previous experiments or empirical knowledge help HyperBand to inform about hyperparameter selection better. While HyperBand with priors samples hyperparameters at random over the search space, it makes use of effective parameter values from other studies and emphasizes portions of the search space, which tends to lead to improved performing configurations. As an example, for a hyperparameter such as learning rate, rather than randomly selecting a value in a certain range just limit the values to be sampled based on some distribution of what the best observed learning rates were from previous trials. Surrogate model is a fast and cheap model that predicts the cost of hyperparameter configuration by not having to retrain full model in every trial, allowing for less computation. Surrogates in HyperBand are used to predict the performance of a new hyperparameter configuration given information from previous configurations.

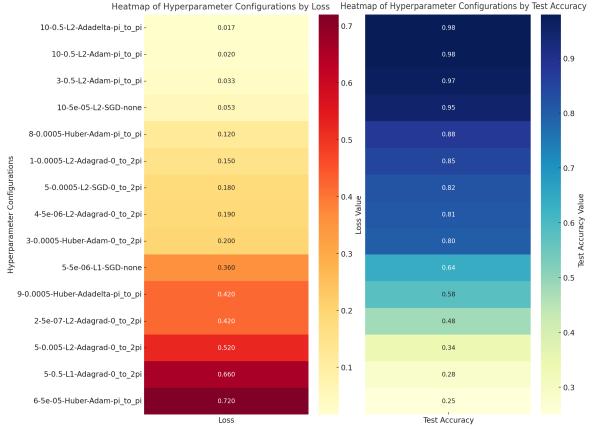


Figure 23: HyperBand optimisation results

The results obtained through the HyperBand optimization method align with those observed using Bayesian optimization. One striking similarity is the recurrence of large learning rates in the optimal configurations. Both methods converge to large learning rate values, which, when combined with adaptive optimizers like Adadelta, Adagrad or Adam, seem to yield the best performance. One difference between the two approaches lies in the inclusion of a new hyperparameter during HyperBand optimization: data normalization. In the Bayesian optimization experiments, this hyperparameter was not considered, meaning that the current results explore an additional dimension of the model’s hyperparameter space. One other key difference is the deepness of the model. HyperBand tends to end up with much deeper optimal configs than the bayesian optimization process favored. This leads to the hypothesis, namely, while learning rate and optimizer are important in steering model performance (at least) hyperparameters such as depth, loss function and even normalization may be less impactful on test accuracy and loss. Thus, it could be that these latter hyperparameters do not have a very significant effect on model performance, as long as learning rate and optimizer are well tuned. Moreover, HyperBand was generally faster than Bayesian optimization in identifying optimal hyperparameter configurations.

This study allows us to investigate the correlations between hyperparameters of the QRU model—specifically depth, learning rate, and optimizer—using heatmaps to highlight combinations that optimize performance in terms of aver-

age loss and test accuracy, revealing that adaptive optimizers paired with moderate learning rates yield the best results.

5 Conclusion

Our study demonstrates that the QRU model is well suited for classification tasks in the context of current NISQ devices, due to its minimal resource requirement and strong classification performances. By systematically exploring and analyzing both model-specific hyperparameters (such as circuit depth, rotation gates and input normalization) and training hyperparameters (including learning rate, batch size, optimizer choice and loss functions), we identified optimal configurations that balance accuracy and computational efficiency, thus making the QRU highly suitable for real-world quantum machine learning applications.

Through the application of global optimization methods, we uncovered significant correlations and interactions among hyperparameters. Moreover, our mathematical analysis established the QRU’s superior expressivity compared to the widely-used VQC. Indeed, we highlighted that VQC’s limitations are not only in terms of qubit counts and entanglement gate noise but also in the expressivity boundaries in Fourier frequency domains. These insights justify the QRU as the preferred choice for quantum machine learning tasks.

This work thus provides a solid framework for optimizing QRU performance within the constraints of current quantum hardware, representing a significant advancement toward their practical application in diverse scientific fields such as including high-energy physics.

Code availability. All code and experimental data supporting the results of this paper are publicly available at: https://github.com/LeaCasse/QRU_Calorimetry_Optimization

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