

How Do Hybrid Quantum-Classical Physics-Informed Neural Networks Learn?

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Abstract

Physics-Informed Neural Networks (PINNs) revolutionized the field of Scientific Machine Learning. The community has explored several variants of PINN. Quantum-Assisted Physics-Informed Neural Network (QAPINN)— a hybrid quantum-classical variant of PINN— was introduced by Shah et al. [7]. QAPINN reduced weights up to 20% as compared to the equivalent classical PINN while improving or maintaining accuracy. In this work, we employ activation maps as an initial explainability tool to investigate how QAPINNs learn and discuss future directions using richer representation analysis techniques. We discuss the effect of introducing a quantum hidden layer on the learning process of a PINN, the role of entanglement and output extraction method, and effect of choice of rotational gates for the variational layers in QAPINN architecture.

1 Introduction

Physics-Informed Neural Networks were introduced in [5] giving rise to the field of Physics-Informed Machine Learning. PINNs are used to solve ODEs/PDEs and estimate the true values of involved constants. They are standard fully connected feed-forward neural networks with modified loss function.

$$\text{Loss} = \lambda_{\text{pde}} \mathcal{L}_{\text{pde}} + \lambda_{\text{IC}} \mathcal{L}_{\text{IC}} + \lambda_{\text{BC}} \mathcal{L}_{\text{BC}} + \lambda_{\text{data}} \mathcal{L}_{\text{data}} \quad (1)$$

A typical NN loss function is Mean Squared Error or Categorical Cross Entropy. However, for a PINN the ODE/PDE being solved becomes the loss function alongside the associated initial and boundary conditions. If data is available, additional data loss term can be added. Multiple Variations of the standard classical PINNs have been explored in the community [1, 2, 4].

Quantum Assisted Physics-Informed Neural Network (QAPINN) represented as

$$u_{\Theta, \theta}(\mathbf{x}) = f_{\theta}(\Phi_{\Theta}(\mathbf{x})), \quad (2)$$

where f_{θ} denotes the classical layers following the quantum layer, Θ are quantum weights and θ are classical weights was introduced in [7]. It was obtained by replacing the first classical hidden layer in a standard PINN architecture with quantum hidden layer.

There have been recent theoretical developments attempting to explain the learning in a pure Quantum Neural Network. Schuld *et al.* [6] showed that variational quantum circuits with data encoding admit a partial Fourier representation, where the encoding determines the accessible frequency spectrum while trainable quantum layers determine the corresponding Fourier coefficients. Kashif and Al-Kuwari [3] explored Hybrid Quantum Neural Networks for multi-class classification problem and empirically demonstrated that trainability depends jointly on the choice of data encoding, ansatz expressibility, and entanglement. While these studies explore significant aspects for QNNs and Hybrid QNNs, none focus particularly on learnability of a Hybrid QNN (or a Hybrid PINN). This work attempts to connect internal representations of the model, architectural circuit choices and observed performance to provide a principled explanation for the observed behavior.

2 Methodology and Results

We solve a representative set of ODEs and PDEs to contribute to the gap in explaining how a QAPINN learns. From our previous experiments, we have observed that the alternate variational layers with circular entanglement (Basic Entangler Layers architecture) is the optimal quantum circuit to solve fluid problems with QAPINN [7]. This circuit architecture is used for all the QAPINN variants of the study.

As an illustration, we discuss some of the results obtained from QAPINN trained on diffusion-reaction equation (Equations 3 and 4). The associated boundary condition (Equation 5) and initial condition (Equation 6) and true solution (Equation 7) are shown below.

$$u_t = u_{xx} + F(x, t), \quad (3)$$

where,

$$F(x, t) = e^{-t} \left(\frac{3}{2} \sin(2x) + \frac{8}{3} \sin(3x) + \frac{15}{4} \sin(4x) + \frac{63}{8} \sin(8x) \right). \quad (4)$$

$$u(-\pi, t) = u(\pi, t) = 0. \quad (5)$$

$$u(x, 0) = \frac{\sin(2x)}{2} + \frac{\sin(3x)}{3} + \frac{\sin(4x)}{4} + \frac{\sin(8x)}{8}. \quad (6)$$

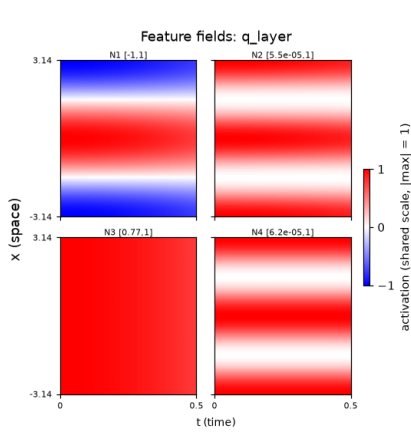
$$u(x, t) = e^{-t} \left(\frac{\sin(2x)}{2} + \frac{\sin(3x)}{3} + \frac{\sin(4x)}{4} + \frac{\sin(8x)}{8} \right). \quad (7)$$

We discuss the results obtained with 4-qubit and 6-qubit QAPINN models. Each model was trained with only physics loss (PDE, boundary condition and initial condition losses), and no data loss was included in training. The obtained best relative L_2 error on validation dataset for 4-qubit and 6-qubit QAPINN architectures with and without entanglement for different rotation gates in the variational layers are displayed in Table 1. The RX rotational gate was used for input embedding for each listed variation and expectation values for Pauli-Z observable was used to extract quantum circuit output.

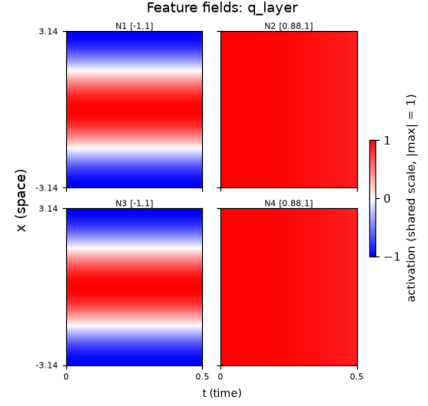
Qubits	With Entanglement			Without Entanglement		
	Rx	Ry	Rz	Rx	Ry	Rz
4	0.0931	0.5966	1.0019	0.0043	1.0006	1.0005
6	0.0256	0.6755	1.0018	0.0057	1.0008	1.0007

Table 1: Relative L_2 error on validation dataset for 4 and 6 qubit QAPINN architectures employing different rotation gates in the variational layers, with and without entanglement

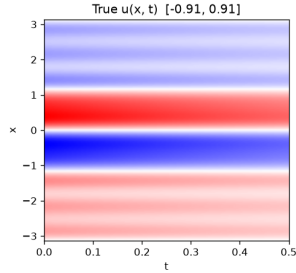
The RX -layer without entanglement variant performs the best for both 4-qubit and 6-qubit QAPINN. As claimed in [3], we verify that entanglement does hurt the performance of a Hybrid Model in physics-informed machine learning setup too for angle input encoding. The RZ -based variants performed the worst. Since RZ commutes with the Pauli-Z readout, coupling the two leaves the variational parameters nearly inert and drags the whole model to relative L_2 near 1. The observable and the variational gate therefore have to be chosen together. Since the largest performance gap is observed between the entangled and unentangled RX -based models, we investigate their learned representations using activation maps. Each activation map visualizes the spatio-temporal feature encoded by an individual qubit and identifies the regions of the solution domain to which that qubit is most responsive. The resulting activation maps for the four-qubit quantum layer, together with the ground-truth solution, are shown in Fig. 1. We observed drastic changes between the activation maps of classical layers of classical PINN and the QAPINN variants. However, due to space constraints we do not include them here.



(a) Quantum layer with entanglement.



(b) Quantum layer without entanglement.



(c) Ground truth solution of the diffusion-reaction equation.

Figure 1: Activation maps on the validation dataset of the 4-qubit quantum hidden layer for QAPINNs with (a) entanglement and (b) no entanglement, together with (c) the ground truth solution of the diffusion-reaction equation.

Figures 1a and 1b demonstrate that introducing entanglement changes the internal feature representations learned by the quantum layer. While both architectures capture structures that resemble components of the ground-truth solution (Fig. 1c), the learned representations differ qualitatively, indicating that entanglement alters the feature extraction process rather than simply improving predictive accuracy. Interestingly, the unentangled model achieved significantly lower validation error despite learning a different set of representations, suggesting that richer quantum correlations do not necessarily translate to better generalization for this problem. These observations motivate a more comprehensive representational analysis using additional explainability techniques, which we outline in the next section.

3 Conclusion and Future Work

The learning mechanisms of hybrid quantum-classical PINNs (QAPINNs), and hybrid neural networks more broadly, have received limited attention in the literature. We discuss the results of 4 and 6 qubit QAPINN architecture on diffusion-reaction equation and illustrate how architectural choices for the quantum circuit largely affects the performance of the entire hybrid model. We further demonstrate how entangled and unentangled circuit-based quantum layers learn different features.

We plan to extend this study to a wider range of ODEs and PDEs. Explainable AI (XAI) techniques such as representation similarity methods (CKA, SVCCA, RSA) will compare learned features, while representation complexity metrics (effective rank, intrinsic dimensionality and singular-value spectra) will quantify feature diversity. Saliency maps will identify influential qubits and activation maps will characterize learned spatio-temporal features.

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