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Variational Quantum Circuit for Classification of a Mock Dataset using Quantum Neural Network

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I. Introduction

Quantum machine learning is a trending topic of research. As the computing capabilities of quantum computers increase, the application field of quantum computing expand. Machine learning can be regarded as a natural candidate for quantum computing. The possibility of "parallel" processing of data aligns well with machine learning concept, where several features can be encoded and processed at the same time. This is especially true for large data sets where there might be 100s of features, which would be difficult to handle with classical computers. Although quantum computers are not capable of working with such datasets yet, there is merit at research on QML using smaller datasets. The understanding, methods, and algorithms developed can be adapted to large data applications in the future.

In this task, a mock train set is provided with 4 features and one dependent variable. The dependent variable is binary labeled. The features are given as integers. A similar dataset is also provided for a mock test for validation of training. A snippet of the mock training data is presented in Fig. 1. In terms of coding, Python language was used in addition to Qiskit, Pandas, sklearn, Numpy, and matplotlib modules.

	0	1	2	3	x
0	2789.26	1000	10	20	0
1	4040.01	1000000	1	1	1
2	2931.20	10000	10000	40	1
3	3896.54	10000	100000	30	1
4	982.06	100	1000	75	0
5	1579.81	1	1000	90	0
6	3031.77	1000000	1000000	35	1
7	860.44	10	100000	60	0

Figure 1. The mock dataset has 4 features (columns 0 to 3) and 1 dependent variable (column x). Data set has not been altered except for the column labeling of the dependent variable. Original variable label (4) is not compatible with some of the syntax required for the Pandas module. Hence it was replaced with label "x".

The task is to use two or more encoding schemes and design accompanying ansatz for variational quantum circuits to classify the mock test dataset. The performance of variational quantum circuit (VQC) is investigated by varying encoding schemes, ansatz design, and layer number of the ansatz. The section II explains the encoding schemes that was used in this study. The ansatz design is presented in Section III. The performance of each VQC design and analysis is given in Section IV. Finally, conclusions are given in Section V.

II. Data Encoding

Encoding of classical data for quantum computing can be achieved via several methods including angle, basis, and amplitude encoding. For this task, three feature maps from Qiskit's circuit library was used, the Z, ZZ, and Pauli. The feature maps, in essence, are angle encoding schemes. The Z feature map is a Hadamard gate followed by a single qubit rotation gate about the Z-axis. The ZZ feature map adds a CNOT and an additional Z-axis rotation on top of the Z feature map. The Pauli feature map is a generalized circuit which could be modified into Z or ZZ feature maps by changing Pauli designations. In this work, Pauli feature map was used with "ZY" designation which forms a circuit with additional X-axis rotations. The major difference between Z feature map is that it does not have entangled qubits unlike the other feature maps. The encoding circuits are presented in Fig. 2.

Prior to encoding, the classical data was analyzed by graphing out the correlation between features versus the variable. Then, four separate arrays were formed from the train and test dataset: a. dataset

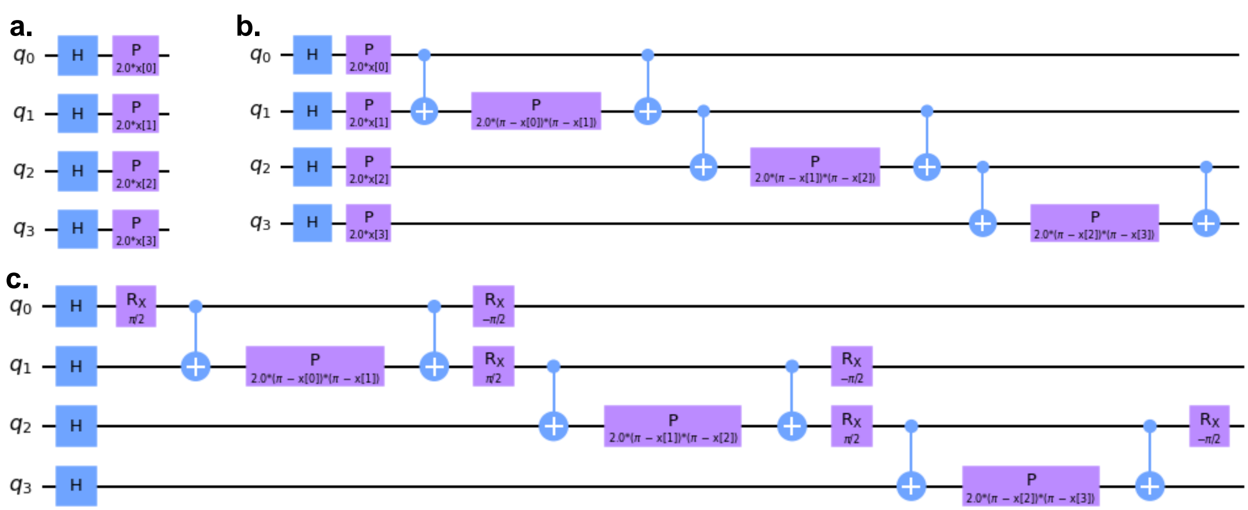

Figure 2. The Z feature map features one Z-axis rotation (P) for each qubit (a). The ZZ feature map entangles adjacent qubit and adds extra Z-axis rotations (b). The Pauli feature map replaces the initial Z-axis rotation gates and adds staggered X-axis rotations (c).

with only independent training values (x_train), b. dataset with only dependent training values/labels (y_train), c. dataset with only independent test values (x_test), d. dataset with only dependent test values/labels (y_test). Next, the x_train and x_test datasets were normalized for each column. Finally, x_train dataset was encoded into the parameterized feature maps.

III. Ansatz Design

Three different ansatz designs are investigated. First, the TwoLocal ansatz from Qiskit circuit library was used in combination with the Z feature map. The results of this combination was used as a reference point for the minimum desired performance.

The two original ansatz designs are shown in Fig. 3. First original design is similar to the TwoLocal ansatz but adds an additional CNOT for a closed ring circuit. It also removes the second set of RY, RZ gates following the CNOT gates. The second original design is a derivative of the first. It removes the Z-axis rotations for all qubits in addition to the closed ring design. The weight parameters were randomly created using a fixed seed to ensure comparability between results.

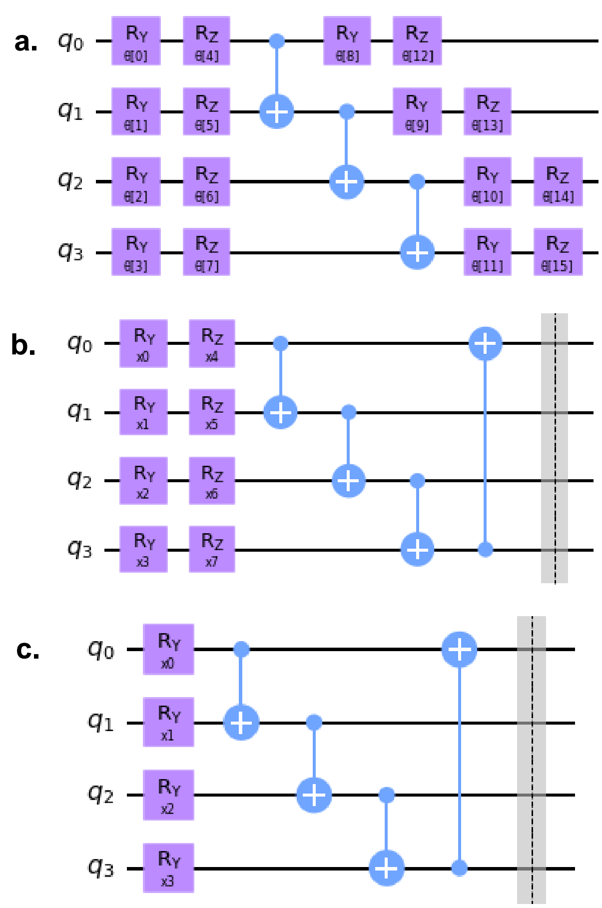

Figure 3. The TwoLocal (a), Custom-1 (b), and Custom-2 (c) ansatz circuits. Here, each circuit is represented as single layer.

IV. Results & Discussion

The performance of all VQC designs were investigated using Qiskit's Aer simulator with 2048 shots. For the training, Quantum Neural Network approach was used. For the optimization, SPSA was used with a fixed 50 iteration limit.

The reference design (Ref) with the Z feature map and TwoLocal ansatz was able to achieve 79.6% training accuracy and 81.6% test accuracy for the 3-layer and 2-layer ansatz circuits. The objective was to design VQCs that can achieve either similar performance with less circuit depth or better performance with similar circuit depth. In addition, the ideal VQC would also converge with less iterations. A summary of all results is shown in Table 1.

The Custom-1 ansatz design showed the better performance with Z feature map compared to other encoding schemes, which was a recurring trend for all VQCs including the reference design. Overall, the best results were achieved for a 3-layer ansatz with 80.6% training and 82.5 test accuracies. Considering that the simulation does not include measurement noise, the circuit depth would not cause the drop in performance. Instead, it is thought that the more complicated encoding schemes would require substantially different ansatz. Hence, the ansatz that worked well with the simpler Z feature map encoding performs worse with ZZ and Pauli feature maps. Another explanation might be the over-training. In author's opinion, this is unlikely and cannot be proved without further trials with different ansatz designs. The impact of number of layers on accuracy had a linear trend for the ZZ and Pauli feature maps where the VQC consistently performed worst with the test set compared to the training set. For the Z feature map, there was slight improvement in the training versus test

Table 1. Summary results for the training and test accuracy of each VQC.

VQC	Accuracy	1-Layer [%]	2-Layer [%]	3-Layer [%]
Ref VQC Z Fmap - TwoLocal	*Train:* *Test:*	54.3 51.6	71.6 81.6	79.6 81.6
VQC 1: Z Fmap – Custom-1	*Train:* *Test:*	58.6 45.8	59.3 43.3	80.6 82.5
VQC 2: ZZ Fmap – Custom-1	*Train:* *Test:*	56 49.1	57 57.5	59 49.1
VQC 3: Pauli Fmap – Custom-1	*Train:* *Test:*	56.6 53.3	61 56.6	64 60
VQC 4: Z Fmap – Custom-2	*Train:* *Test:*	58.6 44.1	53.6 55.8	76.3 83.3
VQC 5: ZZ Fmap – Custom-2	*Train:* *Test:*	52 47.5	52.3 53.3	56.6 54.1
VQC 6: Pauli Fmap – Custom-2	*Train:* *Test:*	55.6 47.5	55.6 54.1	69.3 60.8

accuracy with increasing number of layers. A trial run was done with 4 layers, but it resulted in performance similar to 2-layer design. Hence, it can be concluded that for Custom-1 ansatz with Z feature map, 3 layers is the optimum design.

The Custom-2 ansatz design performed the best in this study. The Z feature map with the Custom-2 ansatz achieved 76.3% training and 83.3% test accuracy (VQC 4). The low performance with the ZZ and Pauli feature maps was evident with the Custom-2 ansatz as it was in the Ref and Custom-1 ansatz VQCs. On the other hand, VQC 4 exhibited better training-to-test accuracy ratio than VQC 1 for 2- and 3-layer designs. Furthermore training-to-test ratio was improved with increasing number of layers unlike in the case of Ref VQC and VQC 1. Hence, a 4-layer trial was conducted to see if a better performance could be achieved. Although the training-to-test (57% vs 63.3%) accuracy ratio was further improved, overall performance was worse. Nevertheless, this suggests that further small tweaks to the ansatz may improve performance.

V. Conclusions

In this task several VQC designs were investigated. The objective was to achieve similar or better performance compared to pre-made ansatz circuit from the Qiskit circuit library. A simple closed ring ansatz with Hadamard and Z-axis rotation gates (VQC 4) was able to outperform the reference design when encoded with the Z feature map. Furthermore, the VQC 4 converged in 29 iterations while the reference VQC converged in 47 iterations. Finally, the VQC 4 ansatz has less circuit depth which would reduce errors in a real quantum computer. Hence, it can be concluded that the task was completed successfully.