Quantum Neural Networks for Analyzing X-Ray Scattering Data

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ABSTRACT

Determining the chemical structures of molecules from scattering cross-sections has been a long-standing problem in chemistry. To date, it is accomplished by performing massive molecular dynamics simulations. To avoid such calculations, researchers have developed Classical Machine Learning (CML) methods. But, the sheer complexity of the problem requires vast Neural Networks and enormous datasets. Quantum Machine Learning (QML) on NISQ computers has shown great potential in dealing with such issues while using exponentially smaller resources. Here, we demonstrate the operation of simple Quantum Neural Network (QNN) architectures that can provide insights into the dataset by using just a few qubits and small sample sizes. We explore various Parameterized Quantum Circuits (PQC), state preparation schemes, and circuit decomposition algorithms. Finally, we present a comparison between the QML and CML approaches.

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Introduction

- **Prediction**: X-ray scattering cross-section (Input) → Molecular Coordinates like Bond Length, Bond Angle, and Dihedral Angle (Output) of N-Methylmorpholine.
- Ultrafast-pulsed X-ray free-electron lasers (**XFELs**) produce scattering data which can be used to observe structural changes in chemicals during reactions.
- The training dataset is obtained from Molecular Dynamics Simulation.
- **Hybrid Quantum-Classical Machine Learning**: QPU evaluates the Parametrized Quantum Circuit, and CPU handles ancillary computations and optimises parameters using Classical Algorithms.
- Data Pre-processing: Principal Component Analysis (**PCA**) and Scaling.

Figure 1. Predicting Molecular Coordinates (following the Z-matrix representation) from X-ray cross-sections (3 examples).

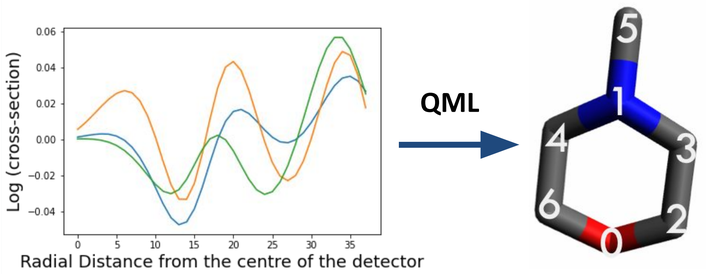
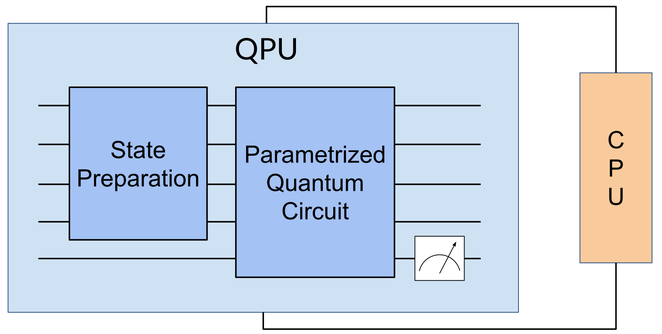


Table 1. Comparison between CML and QML

	Quantum ML	Classical ML	Small CML
Architecture	7-qubit parameterized unitary gate	Three Hidden layers: 475 perceptrons	Three Hidden layers: 50 perceptrons
Sample Size	1000	~ 1 million	1000
Trainable Parameters	168	~ 470,000	~7,000
Epochs	8	100	100
Learning Rate	0.01	1e-4	1e-4

Figure 2. Hybrid Quantum-Classical Neural Network Architecture



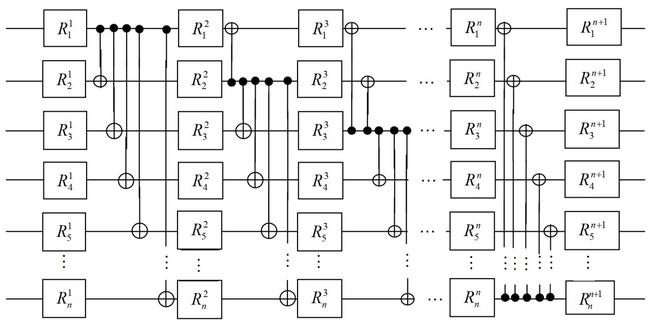
Computational Details

- State Preparation (**Amplitude Encoding**) - The classical information is encoded as the amplitude of the qubits.

$$\vec{x} \equiv (x_0, x_1, x_2, ...x_n) \longrightarrow |x\rangle = \sum_{i=1}^{\log n} x_i |i\rangle$$

- Quantum Neural Network: General **n-qubit Unitary Gate** is used here, but I tried other networks including a **QCNN** circuit.
- Circuit Decomposition - Simplification of huge unitary operations in terms of universal single-qubit unitary and CNOT gates. We use **Sine-Cosine Decomposition**.
- Programming Libraries: **TensorFlow Quantum**, Cirq, and Qiskit.

Figure 3. Parametrized n-Qubit Unitary Rotation Gate



Results and Discussion

- Tested the algorithm by predicting Quantum Fourier Transform.
- **Barren Plateau Problem**: Random initialisation of Quantum Gate parameters lead to vanishing gradients. We use **Identity Block Initialisation** to overcome it.
- Scalability: All the calculations were performed on classical simulators. The Quantum computers currently available are too **noisy**, can handle only small number of qubits and have small coherence time.
- Interestingly our QML algorithms learns insights in the datasets even with so few qubits and a small dataset.
- Encoding classical data into qubits is extremely slow. Hopefully invention of a **QRAM** in the future will help overcome this problem.

Figure 4. Prediction accuracy Heat Map of distance between Oxygen and Nitrogen by (a) CML (b) QML (Architectures mentioned in Table 1). The black-line shows ideal accuracy.

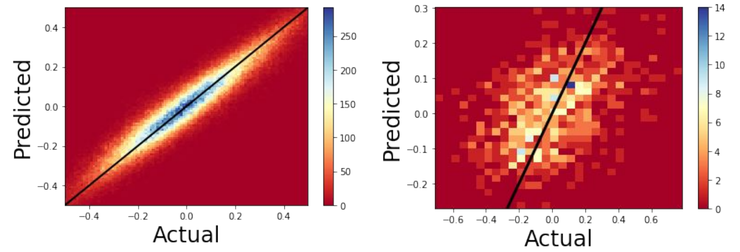


Table 2. Mean R^2-values of Different Neural Network Architectures over Molecular Coordinates.

	Bond Length	Bond Angle	Dihedral Angle
Classical Neural Network (CNN)	0.917	0.994	0.983
Quantum Neural Network (QNN)	0.220	0.277	0.278
Small CNN.	0.189	0.257	0.054

References

- Wolf, T.J.A., Sanchez, D.M., Yang, J. et al. Nat. Chem. 11, 504–509 (2019).
- S. C. Iris Cong and M. D. Lukin, Nat. Phys.15, 1273(2019).
- J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost,N. Wiebe, and S. Lloyd, Nature 549, 195 (2017).
- M. Plesch and Brukner, Phys. Rev. A83, 032302 (2011).
- R. Iten, R. Colbeck, I. Kukuljan, J. Home, and M. Christandl, Phys. Rev. A93, 032318 (2016).
- P. B. M. Sousa and R. V. Ramos, Quantum Info. Comput.7, 228–242 (2007).
- G. Verdon, M. Broughton, J. R. McClean, K. J. Sung, R. Babbush, Z. Jiang, H. Neven, and M. Mohseni, (2019), arXiv:1907.05415 [quant-ph].
- G. Verdon, M. Broughton, and J. Biamonte, (2017), arXiv:1712.05304 [quant-ph].
- R. Sweke, F. Wilde, J. Meyer, M. Schuld, P. K. F¨ahrmann,B. Meynard-Piganeau, and J. Eisert, "Stochastic gradient descent for hybrid quantum-classical optimization,"(2019), 1910.01155 [quant-ph].