Materials Science & Engineering Thesis Defense

Classifying High Entropy Alloys with Quantum Machine Learning

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Abstract

With the abundance of increasingly large datasets, the ability to predict the phase of high-entropy alloys (HEAs) based solely on elemental composition could become a reliable tool for the discovery of new HEAs. However, as the amount of data expands so does the computational time and resources required to train predictive classical machine learning models. Quantum computers, which use quantum bits (qubits), could be the solution to overcoming these demands. Their ability to use quantum superposition and interference to perform calculations could be the key to handling large amounts of data. In this work, a hybrid quantum-classical machine learning algorithm is implemented on both quantum simulators and quantum processors to perform the supervised machine learning task. Their feasibility as a future tool for HEA discovery is evaluated based on the algorithm's performance. An artificial neural network (ANN), run by classical computers, is also trained on the same data for performance comparison. The accuracy of the quantum-classical model was found to be comparable to the accuracy achieved by the classical ANN with a slight decrease in accuracy when ran on quantum hardware due to qubit susceptibility to decoherence. Future developments in the applied quantum machine learning method are discussed.

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