Approximated Quantum Spectral Clustering With Weighted Kernel PCA Method Based on Geometric Quantum Neural Network

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Abstract

Spectral clustering is an unsupervised learning method known for its outstanding performance on datasets with non-linear cluster distributions. Although it is computationally costly, some tractable and useful properties from the problem definition have led researchers to develop a wide range of its variants, depending on applications and purposes. The approach of the weighted kernel principal component analysis (PCA) method is one of such variants. By introducing concepts of kernel PCA into the original spectral clustering problem, the problem can be formulated as a least-square support vector machine (LS-SVM) problem in its primal form, which eventually turns out that its dual problem is an eigen-decomposition problem of a non-symmetric matrix.

In the field of quantum machine learning, the advent of variational quantum algorithms (VQAs) has attracted significant attention from researchers. Although the theoretical advantages of VQAs are still an open question, various interesting algorithms have been proposed as approximation schemes. In particular, the methodology of approximating Lagrangian multipliers with variational quantum circuits mitigates the infeasibility of the original quantum support vector machine problem, allowing machine learning tasks to run on noisy intermediate-scale quantum (NISQ) devices. Furthermore, the design of the template for the variational quantum circuit, known as an ansatz, has become more sophisticated. The geometric quantum neural network (GQNN) is a design method that allows the ansatz circuit to consider the dataset's symmetric structure with prior knowledge provided by algorithm designers. Using the GQNN offers various advantages, such as robustness to barren plateaus and better generalization performance.

In this work, we propose an approximate spectral clustering method that runs on noisy quantum devices. The algorithm is based on the theories of weighted kernel PCA and GQNN. As an approximation scheme, it achieves a polynomial-time speedup compared to classical methods by allowing a small error. We will examine the impacts of the introduced methodologies, which are expected to guarantee better performance in learning compared to naïve approaches with random ansatz circuits which are not GQNN.

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