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Structure Learning for Quantum Kernels

Kernel methods are used in Machine Learning to enrich the feature representation of data in order to improve the generalization property of models. Quantum kernels efficiently implement complex transformations encoding classical data in the Hilbert space of a quantum system. Working with quantum kernels may produce benefits with respect to classical models. However, the choice of a best-performing quantum embedding requires prior knowledge of the data which is typically not available. We propose an algorithm that automatically selects the best quantum embedding through a combinatorial optimization procedure that operates on the structure of the circuit representing the quantum embedding. The algorithm modifies the generators of the gates, their angles (which depend on the data points), and the qubits on which the various gates act in search of the best structure. Since combinatorial optimization is computationally expensive, we have introduced a criterion based on the exponential concentration of kernel matrix coefficients around the mean to immediately discard an arbitrary portion of solutions that may perform poorly. Contrary to the gradient-based optimization (e.g. trainable quantum kernels), our approach is by construction immune from the barren plateau problem. We demonstrate the increased performance of our approach, with respect to randomly generated quantum embeddings, on both artificial and real-world datasets. A more detailed description of this algorithm, the experiments and their results can be found in:

Incudini, M., Martini, F., Di Pierro, A.: Structure Learning of Quantum Embeddings. arXiv (2022). https://doi.org/10.48550/ARXIV.2209.11144. https://arxiv.org/abs/2209.11144

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Short summary of your poster content

The Structure Learning algorithm automatically identifies a satisfactory quantum circuit to be used in machine learning tasks. The algorithm is based on a combinatorial optimization process; numerical properties unique to kernel methods (e.g. concentration of kernel coefficients around an average value) are used to speed up the optimization process.

Poster printing

Yes

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