

Scalable Hardware-Aware Quantum Feature Map Search for Quantum Kernel Learning

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Abstract

Quantum kernel methods use data-dependent quantum circuits to embed classical data into quantum feature spaces, where the induced kernel is processed by a classical learning algorithm such as a support vector machine [1, 2]. Their performance depends strongly on the choice of quantum feature map, since different encodings can induce substantially different similarity geometries even when the downstream classifier is unchanged. In this work, we formulate quantum feature-map construction as a supervised, hardware-constrained architecture search problem.

We propose Quantum Feature Map Search (QFMS), an automated framework for discovering dataset-adapted quantum encodings under explicit restrictions on qubit count, circuit depth, native gate alphabet, and device connectivity. Candidate feature maps are represented as discrete chromosomes encoding gate placements, fixed rotations, feature-dependent rotations, entangling operations, and a global bandwidth parameter controlling the scale of data injection. Each chromosome is decoded into a hardware-compliant quantum circuit, used to construct the fidelity kernel $K_\chi(x_i, x_j) = |\langle \psi_\chi(x_i) | \psi_\chi(x_j) \rangle|^2$, and scored through an SVM-derived loss computed from the resulting precomputed kernel matrix. A genetic algorithm then explores the constrained circuit space using selection, crossover, mutation, and repair operators that preserve executable encodings throughout the search, directly optimizing the task-dependent kernel geometry rather than an abstract circuit expressivity measure.

The framework is evaluated through a staged experimental protocol covering a group-structured benchmark inspired by covariant quantum kernels [3], the high-dimensional Madelon synthetic dataset, and the HIGGS real-world classification dataset from high-energy physics. This progression is intended to test whether automated feature-map search can move from recovering structured inductive biases to constructing useful encodings for nonlinear synthetic and real-world tabular data. We also introduce a transfer-expansion strategy in which feature maps discovered under smaller qubit and depth budgets are embedded into larger circuit families, providing a route toward larger hardware-aware quantum kernels. Rather than presenting quantum advantage claims, the objective of this work is methodological: to provide a systematic route for constructing quantum kernels that are dataset-adapted, hardware-aware, and comparable against classical kernel baselines under a consistent evaluation protocol, complementing recent work on quantum kernels, bandwidth selection, and quantum architecture search [4, 5].

References

- [1] M. Schuld and N. Killoran, “Quantum machine learning in feature Hilbert spaces,” *Physical Review Letters*, vol. 122, no. 4, 040504, 2019.
- [2] V. Havlíček et al., “Supervised learning with quantum-enhanced feature spaces,” *Nature*, vol. 567, pp. 209–212, 2019.
- [3] J. R. Glick et al., “Covariant quantum kernels for data with group structure,” *Nature Physics*, vol. 20, pp. 479–483, 2024.
- [4] R. Shaydulin and S. M. Wild, “Importance of kernel bandwidth in quantum machine learning,” *Physical Review A*, vol. 106, 042407, 2022.
- [5] D. Martyniuk, J. Jung, and A. Paschke, “Quantum Architecture Search: A Survey,” *arXiv:2406.06210*, 2024.