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QCBM Improves the Performance of Classification Based on Some Graph Kernels

We employ QCBM to enlarge molecular datasets with artificially generated samples for training SVMs to enhance the classification performance of selected kernel methods. Quantum Circuit Born Machine have been observed to be an effective tool for neural networks[LW18, oth25, Plo26]. Generative quantum machine learning has attracted significant interest as a potential application of near-term quantum devices. Among the most widely studied models are Quantum Circuit Born Machines (QCBMs)[L⁺22, LW18, S⁺23], which learn probability distributions through parameterized quantum circuits and Born-rule sampling. Most studies evaluate QCBMs using generative metrics such as fidelity, KL divergence, or maximum mean discrepancy (MMD). However, a central question remains largely unexplored: can quantum-generated samples improve predictive models? In this work, we investigate the use of QCBM-generated synthetic molecular data for augmenting graph-kernel classifiers. We study the approach on different datasets including on blood-brain barrier permeability prediction, an important task in early-stage drug discovery.

More broadly, We study whether a *quantum circuit Born machine* (QCBM) can be used as a generative augmenter for kernel-based molecular graph property prediction, and we propose to drive its training with a *graph-spectral* kernel. In our work we carry out a comprehensive study of QCBM enlarged training datasets for data relevant in molecular biology and chemistry research. In particular we test the performance of two previously introduced topology-based graph kernels[WE25, WWE25]. We observe classification accuracy enhancements on most datasets, and find that QCBM works particularly well for the effective resistance graph kernel introduced in[WE25].

Concretely, we represent each graph by a fixed-length descriptor of its pairwise *effective resistances*, derived from the pseudo-inverse of the graph Laplacian, and build an RBF kernel over these descriptors. A QCBM is then trained to match the data distribution in this effective-resistance (ER) feature space by minimising a maximum mean discrepancy (MMD) objective evaluated with the ER kernel. Generated bitstrings are mapped into ER space through a learned linear read-out and appended to the training set of a kernel ridge regressor (property regression) and an SVM (activity classification). On a controlled synthetic benchmark mirroring the topology of AIDS/PROTEINS/NCI1, ER-kernel-guided QCBM augmentation preserves baseline regression quality ($\text{RMSE} = 2.40$, $R^2 = 0.77$) and consistently improves on structure-agnostic random augmentation ($\text{RMSE} = 2.46$, $R^2 = 0.76$), while the ER-MMD objective decreases monotonically during training. All results use a classical simulation of the Born machine.

Our contribution is the coupling of a topology-aware spectral kernel with the MMD training of a Born machine for graph-structured data. And we observe substantial improvements on practical datasets, indicating that QCBM has the capability to substantially boost the performance of the selected graph kernels.

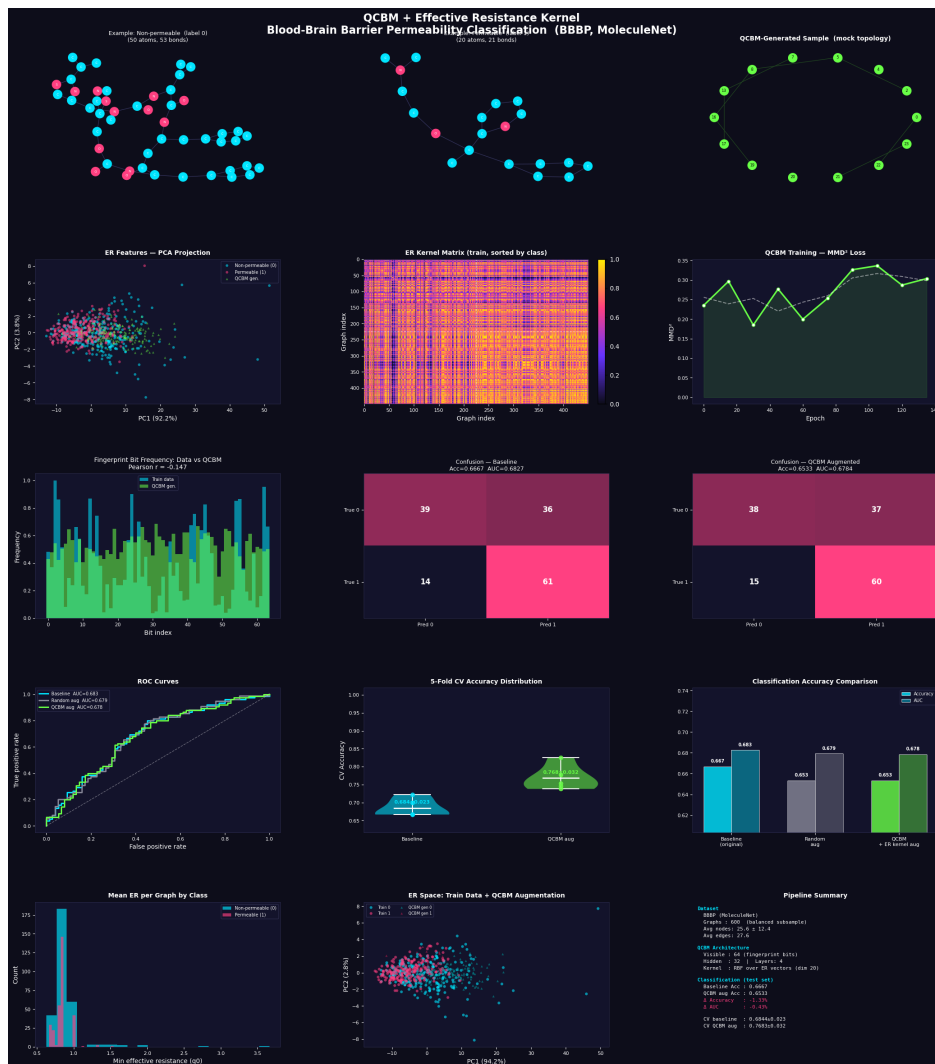


Figure 1: Results of the benchmark of the QCBM applied to improve the classification accuracy of the effective resistance kernel.

References

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