Efficient computation of the Gram matrix of eigenvectors for quantum kernel methods

Abhijeet Alase[1], Salini Karuvade[1], and Hari Krovi[2]
[1] *School of Physics, University of Sydney, Sydney, New South Wales 2006, Australia*
[2] *Riverlane Research, Cambridge, MA*

In quantum kernel methods, the possible choices for the kernel function are limited by the form of the feature map, which in turn is specified by a quantum circuit parametrized by the classical data. Developing quantum algorithms for the computation of novel kernels is an important problem in the field of quantum machine learning. In this work, we construct an efficient quantum algorithm for computing any given element of the Gram matrix of the eigenvectors of a given diagonalizable, possibly non-Hermitian, matrix with real spectrum. Our algorithm leverages a novel formula for expressing this Gram matrix in terms of the given matrix and its adjoint. The design of our algorithm combines results from the theory of PT-symmetric quantum mechanics and tools from the block-encoding framework for quantum linear algebra. If the classical data is embedded in the eigenstates of a diagonalizable operator with real spectrum, then the Gram matrix of the eigenstates is the quantum kernel, a description of which is efficiently computed by our algorithm. Thus, our work prompts the exploration of quantum feature maps beyond those specified by parametrized quantum circuits.