Quantum computing for kernel methods

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While the majority of approaches in quantum machine learning focus on neural network-based models, the basic idea of quantum computing is actually surprisingly similar to that of *kernel methods* in machine learning, such as the support vector machine. Both quantum computing and kernel methods can be understood as a way to efficiently perform computations in an intractably large Hilbert space. In quantum computing, a vector Ψ from a "quantum" Hilbert space represents the state of the quantum system which is manipulated by a quantum algorithm. For qubit-based systems this quantum Hilbert space grows exponentially with the size of the quantum computer, and so-called continuous-variable quantum computers even have an infinite-dimensional Hilbert space for very small quantum computers. In machine learning, Hilbert spaces play the role of feature spaces in which data gets mapped in order to be analysed with relatively simple models. However, instead of performing the mapping explicitely, kernels - inner products of vectors in feature space - are used to build classifiers for supervised learning.

We show how this analogy can be leveraged to design machine learning algorithms that make use of quantum computers. For this we propose to prepare the quantum computer in a state $\Psi(x)$ that depends on a vector of input features x. This effectively maps the features to the quantum Hilbert space, which serves as a feature space for the data. We show how quantum algorithms can be used to implement classifiers which find patterns of data mapped to the quantum feature space.

As a specific example we propose one particularly simple way of building a "quantum-enhanced classifier" that suits noisy and small-scale early-generation quantum computing technologies. The quantum device is used to estimate inner products $\langle \Psi(\mathbf{x}), \Psi(\mathbf{x}') \rangle$ of quantum states prepared from different inputs. These inner products are interpreted as a custom kernel that can be plugged into models like a support vector machine. We give an example for a continuous-variable quantum computer and show in simulations that it can in principle generate kernels which can be used for supervised learning.

As an outlook, we discuss the important question whether there are kernels which lead to powerful classifiers, but which are not possible to simulate on a classical computer. This would be a demonstration that quantum computing can make a worthwhile contribution to machine learning which is in the reach of near-term quantum devices.

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