Quantum Graph Machine Learning on a Neutral Atom Processor

Lucas Leclerc

Pasqal

lucas.leclerc@pasqal.com

The manipulation of neutral atoms by light is at the heart of countless scientific discoveries in the field of quantum physics in the last three decades. The level of control that has been achieved at the single particle level within arrays of optical traps, while preserving the fundamental properties of quantum matter (coherence, entanglement, superposition), makes these technologies prime candidates to implement disruptive computation paradigms. For instance, using such a quantum processor to embed and process classical data enables the generation of correlations between variables that are inefficient to represent through classical computation. A fundamental question is whether these correlations could be harnessed to enhance machine learning performances on real life datasets.

To that end, we introduce a quantum feature map to encode the information about graphs in the parameters of a tunable Hamiltonian acting on an array of qubits. Using this tool, we first show that interactions in the quantum system can be used to distinguish non-isomorphic graphs that are locally equivalent. We then realize a toxicity screening experiment, consisting of a binary classification protocol on a biochemistry dataset comprising 286 molecules of sizes ranging from 2 to 32 nodes, and obtain results which are comparable to those using the best classical kernels. Using techniques to compare the geometry of the feature spaces associated with kernel methods, we then show evidence that the quantum feature map perceives data in an original way, which is hard to replicate using classical kernels.