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Enhancing Quantum Annealing Performance for the Molecular Similarity Problem

Quantum annealing is a promising technique which leverages quantum mechanics to solve hard optimization problems. In this work, we present a quantum annealing approach to measure similarity among molecular structures. In order to overcome the limited hardware connectivity, a problem must be reformulated using minor-embedding techniques. Using a real data set, we investigate the performance of a quantum annealer in solving the molecular similarity problem. We provide experimental evidence that common practices for embedding can be replaced by new alternatives which mitigate some of the hardware limitations and enhance its performance. Common practices for embedding include minimizing either the number of qubits or the chain length, and determining the strength of ferromagnetic couplers empirically. We show that current criteria for selecting an embedding do not improve the hardware's performance for the molecular similarity problem. Furthermore, we use a theoretical approach to determine the strength of ferromagnetic couplers. Such an approach removes the computational burden of the current empirical approaches, and also results in hardware solutions that can benefit from simple local classical improvement. Although our results are limited to the problems considered here, they can be generalized to guide future benchmarking studies.