Does the structure of the QUBO problem affect the effectiveness of quantum annealing? An empirical perspective

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Abstract

In recent years there has been a significant interest in exploring the potential of Quantum Annealers (QA) as heuristic solvers of Quadratic Unconstrained Binary Optimization (QUBO) problems. Some problems are more difficult to solve on QA and understanding why is not straightforward, because an analytical study of the underlying physical system is intractable for large QUBO problems. This work consists in an empirical analysis of the features making a QUBO problem difficult to solve on QA, based on clusters of QUBO instances identified with Hierarchical Clustering. The analysis reveals correlations between specific values of the features and the ability of QA to solve effectively the instances. These initial results open new research opportunities to inform the development of new AI methods supporting quantum computation (e.g., for minor embedding or error mitigation) that are better tailored to the characteristics of the problem, as well as to develop better QUBO formulations for known problems in order to improve the quality of the solutions found by QA. [1]

Keywords

quantum computing, quantum annealing, optimization,

1. Introduction

Quantum Annealers (QA) are heuristic solvers of Quadratic Unconstrained Binary Optimization (QUBO) problems. It is known that some problems are more difficult to solve effectively with QA compared to other ones. However, it's challenging to study analytically the Hamiltonian for large QUBO problems and it is often not clear how to use these findings to develop new general QUBO formulations that are easier to solve on QA. Furthermore, AI techniques based on the characteristics of QUBO problems able to support QA, such as for minor embedding or error mitigation, are lacking, since the characteristics which represent the difficulty of a QUBO problem are unknown.

In this work, we study with an empirical perspective the characteristics making a QUBO problem difficult to solve on QA, in particular when it requires too many qubits for the analytical study of the Hamiltonian, trying to answer to the question: does the structure of a QUBO problem affects the effectiveness of QA?

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2. Methodology and Experimental Pipeline

In this study we consider instances of the Maximum Cut, Minimum Vertex Cover, Graph Coloring, Set Partitioning, Number Partitioning problems [1]. Each instance has 30-32 QUBO variables, corresponding to 100-150 qubits on the physical embedding of QA. For all instances we compute several features based on the energy distribution of their solutions and on the spectral representation of the QUBO problem as a graph. In particular, the **Spectral Flatness** measures the uniformity of the spectrum of the distribution of the solutions of a QUBO instance [2]; the **Graph Spectral Flatness** measures the uniformity of the spectrum of a signal on a graph [3], when both the signal and the graph are related to the same QUBO instance.

All instances are solved with the D-Wave Advantage QA and also with Simulated Annealing and Tabu Search, considered as baseline methods. Instances are then clustered on the base of their features and the clusters are validated with Silhouette Coefficient. In order to corroborate the obtained results, we also include four test instances related to the Feature Selection problem [4] and check to which cluster they are closest to, according to the computed features.

3. Results and Discussion

The analysis reveals correlations between the clusters and the ability of QA to solve the instances effectively. In particular, we see that instances characterized by high levels of Spectral Flatness are solved optimally by QA. Furthermore, we see also that instances which have low levels of Graph Spectral Flatness are solved optimally too by the QA.

All these findings are corroborated by the test instances we have considered, confirming the relationship between the quality of the solution found by the QA and the structure of the QUBO problem. These initial results open new research opportunities to inform the development of new AI methods supporting quantum computation that are better tailored to the characteristics of the problem, as well as to develop better QUBO formulations for known problems in order to improve the quality of the solutions found by QA.

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