

Avoiding Invalid Quantum State in HOBO for Advancing Traveling Salesman Problem

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In the study of the Traveling Salesman Problem (TSP) using quantum computers, the well-known Quadratic Unconstrained Binary Optimization (QUBO) formulation [1] is often a primary choice. However, due to its high demand for quantum bits, researchers have proposed a more efficient Higher Order Binary Optimization (HOBO) formulation, which reduces the required number of qubits from $O(N^2)$ to $O(N \log N)$ [2]. Despite this improvement, both methods rely on penalty functions that involve two constraint terms [3]. Building on this foundation, we propose a novel encoding approach that reduces the number of constraints. By leveraging this approach, we can effectively eliminate invalid terms.

Here, we focus on detailing how to implement our proposed optimization method. First, in the HOBO formulation, a binary encoding approach is employed to convert decimal numbers into binary representations. For example, a 3-bit binary number can represent 8 states, with each state corresponding to a city node, as illustrated in Figure 1. Taking the TSP with 5 nodes as an example, the original HOBO formulation in Fig.1 (a) requires considering two constraints: one to ensure the validity of the current city node and the other to avoid visiting the same city twice. In our proposed new HOBO formulation in Fig.1 (b), we reformulate the invalid nodes in the first constraint to ensure compliance with the required conditions. By following a sequential order, these invalid nodes are systematically identified and replaced with valid ones.

In this experiment, we continued to utilize the Variational Quantum Eigensolver (VQE) algorithm in quantum computing [4]. For simulation purposes, we used the "aer_simulator_matrix_product_state" available in the Qiskit library [5]. Regarding the preparation of TSP, the coordinates of each city were randomly generated as integer values within a 100×100 matrix, these coordinates were then used to compute a distance matrix [6]. For a 5 nodes TSP, using the NFT optimizer [7], known for its fast convergence with a two-local quantum circuit [6], which incorporate quantum entanglement, our proposed HOBO formulation achieved an accuracy of 0.96. Additionally, it successfully identified the optimal path in 4 out of 10 instances, whereas the original HOBO formulation failed to satisfy the constraint conditions. Under the SU2 quantum circuit [5], the proposed HOBO formulation also demonstrated superior accuracy of 0.87, compared to the original 0.83. These results indicate that our new HOBO formulation better adheres to the constraint conditions and effectively reduces the challenges associated with balancing constraint strength.

(a) Conventional Constraint

Quantum State	$ 0\ 0\ 0\rangle$	$ 0\ 0\ 1\rangle$	$ 0\ 1\ 0\rangle$	$ 0\ 1\ 1\rangle$	$ 1\ 0\ 0\rangle$	Invalid Nodes		
Encoding Node	City 0	City 1	City 2	City 3	City 4	City 5	City 6	City 7

(b) Proposal No Constraint

Quantum State	$ 0\ 0\ 0\rangle$	$ 0\ 0\ 1\rangle$	$ 0\ 1\ 0\rangle$	$ 0\ 1\ 1\rangle$	$ 1\ 0\ 0\rangle$	Reformulated Nodes		
Encoding Node	City 0	City 1	City 2	City 3	City 4	City 0	City 1	City 2

Fig. 1 Comparison of HOBO encoding methods for a 5-node TSP. (a) The original HOBO encoding formulation with invalid constraint. (b) Our proposed new HOBO encoding formulation without invalid constraint.

References

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