QAOA versus Quantum Annealing on Traveling Salesman Problem

...,[1,2] Yongcheng Ding,[1,2,*] and ...

[1] *International Center of Quantum Artificial Intelligence for Science and Technology (QuArtist) and Department of Physics, Shanghai University, 200444 Shanghai, China*

[2] *Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*

(Dated: July 19, 2019)

to be written at the end

I. INTRODUCTION

to be written at the end

II. MODEL

Here we introduce Traveling Salesman Problem (TSP), as the benchmark problem in this paper. TSP sets the goal of answering the following question: what is the most economical route for a traveling salesman that visits its each sites only once and returns to the starting point. This combinatorial optimization problem is proved to be NP-hard, which is notorious for its difficulty to be solved exactly. Even the verification version of TSP, i.e. , checking if there exists any better solution than a given one, is NP-complete. The simplest TSP would be an undirected complete graph, where each edge is weighed by the distance between its nodes. This model could be extended to more complicated cases, e.g., the nodes are not fully connected, or the graph is oriented. Suppose that there are n sites in a d-dimensional space $\mathcal{R}^d$, the distance d_{ij} between site i and j is defined by a certain metric. A weight coefficient w_{ij} represents the cost for a unit distance of d_{ij}, which allows asymmetry of the graph. One can encode the configuration of an arbitrary solution by $n \times n$ binary variables $x_{i,s}$, where $x_{i,s} = 1$ or 0 means "site i is/isnot visited at step s" . The solution is constrained in these ways: (i) only one site can be visited in a single step; (ii) all sites should be visited for only one time in the route.

Accordingly, TSP can be formulated as a 0-1 programming problem for minimizing the total cost

$$\text{cost}(x_{i,s}) = \sum_{i,j,s}^{n} d_{ij} w_{ij} x_{i,s} x_{k,s+1}, \tag{1}$$

$$\text{s.t.} \sum_{i}^{n} x_{i,s} = 1 \text{ for all } s, \tag{2}$$

$$\sum_{s}^{n} x_{i,s} = 1 \text{ for all } i, \tag{3}$$

$$x_{i,1} = x_{i,n+1} \text{ for all } i. \tag{4}$$

A periodic boundary condition Eq. 4 takes the cost for traveling from the last site to the starting point into consideration without introducing extra binary variables. Since the problem is NP-hard, the computing time of any classical algorithm for the worst scenario increases exponentially with the number of sites.

III. QUANTUM OPTIMIZATION ALGORITHM

For problems that cannot be solved by classical algorithms efficiently, quantum computing is applied to speed up the calculation by the principle of quantum mechanics. Among all quantum algorithms, there are quantum optimization algorithms that minimize a given cost function, where is modeled by a combinational optimization problem in this paper. The core idea is that, one may substitute an arbitrary classical binary variable x by qubit operator $\hat{q}$ with eigenvalues of 0 and 1, i.e., $\hat{q}|0\rangle = 0$ and $\hat{q}|1\rangle = 1$ and accelerate the calculation by superpositions and coherence. In this way, the cost function is transformed to a problem Hamiltonian, where its ground state gives the global minimum.

A. Problem Hamiltonian

As we mentioned in Sec. II, the configuration of a certain solution can be encoded by $n \times n$ binary variables, which requires at least the same amount of qubits for the implementation in a quantum computing platform. Much more computational resource can be included as ancilla qubits for achieving error-correction or qubits are not connected according to the graph structure of the problem Hamiltonian.

The problem Hamiltonian can be constructed by additional quadric penalty terms with adequate penalty strengths that represent constraint conditions. For a TSP, the total cost can be translated to a sub-Hamiltonian with the combination of Eq. 1 and 4

$$H_{\text{cost}} = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{s=1}^{n-1} d_{ij} w_{ij} \hat{q}_{i,s} \hat{q}_{j,s+1} + \sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij} w_{ij} \hat{q}_{i,1} \hat{q}_{j,n}, \tag{5}$$

where qubit operator $\hat{q}_{i,s}$ denotes the status of site i in step s. Constraint conditions Eq. 2 and 3 can be ex-

* jonzen.ding@gmail.com

pressed by penalty terms

$$H_{\text{penalty}} = \sum_{s=1}^{n} \lambda_s (\sum_{i=1}^{n} \hat{q}_{i,s} - 1)^2 + \sum_{i=1}^{n} \mu_i (\sum_{s=1}^{n} \hat{q}_{i,s} - 1)^2, \quad (6)$$

where penalty strength λ_s and μ_i should ensure that any action that violates the constraint conditions will lead to a penalty larger than the reward from the total cost. Hence, the problem Hamiltonian can be given by $H_{\text{P}} = H_{\text{cost}} + H_{\text{penalty}}$, with its ground state to be the global minimum we want to obtain by quantum optimization algorithms.

B. Quantum Approximated Optimization Algortithm

We briefly review Farhi's original protocol of QAOA before our mapping. QAOA is an approximated algorithm based on quantum circuit for combinatorial optimization problem, e.g., MAXCUT, MAX-2-SAT, etc. To be more specific, this algorithm maximize a cost function $C(z)$, where $z = z_1 z_2 \cdots z_n$ is a bit string with $z_i = \pm 1$ approximately via a sequence of unitary operators. Once we choose the computational basis vector $|z\rangle$, two unitary operators can be defined by $U(B, \beta) = \exp(-i\beta B)$ and $U(C, \gamma) = \exp(-i\gamma C)$, where $B = \sum_i^n \sigma_x$ is the sum of n Pauli-X operators. Angle β and γ as independent parameters in $[0, 2\pi]$ and $[0, pi]$, respectively. The initial state is prepared to be a uniform superposition $|s\rangle = |+_i +_2 \cdots +_n\rangle$, which is the ground state of B. An angle dependent quantum state can be evolved according to $2p$ unitary operators

$$|\beta, \gamma\rangle = U(B, \beta_p) U(C, \gamma_p) \cdots U(B, \beta_1) U(C, \gamma_1) |s\rangle, \quad (7)$$

where the expectation value of C can be measured by $F_p = \langle \beta, \gamma | C | \beta, \gamma \rangle$. For a fixed accuracy p, the set of angles (β, γ) can be altered to obtain a better F_p. The maximum value of F_p is always larger than that of F_{p-1}, and when $p \to \infty$, this algorithm gives an exact global maximum.

For solving TSP by QAOA, the problem Hamiltonian should be reformulated to fit this protocol. Since the problem Hamiltonian C for QAOA is a spin-1/2 Hamiltonian, qubit operators can be substituted by Pauli-Z operators with $\hat{q}_{i,s} = (1 + \hat{\sigma}_{i,s}^z)/2$. The spin-1/2 Hamiltonian H_{spin} is to be minimized, while QAOA is designed for maximize the problem Hamiltonian C. An effective problem Hamiltonian to be maximized can be generated by $C = -H_{\text{spin}}$.

C. Quantum Annealing

Quantum annealing is another approach to accelerate computation of specific problems by the principle of quantum mechanics. A more precise description of the algorithm would be adiabatic quantum computation (AQC), where a quantum system is initially prepared to the ground state of a simple Hamiltonian and then adiabatically evolved to the problem Hamiltonian. The system is supposed to be in the ground state of the problem Hamiltonian at the end, which is guaranteed by the adiabatic theorem. The estimation of evolving time $t_f = O(1/\text{gap}_{\text{min}}^2)$ is governed by the minimal energy gap of the problem Hamiltonian. The Hamiltonian of the quantum system can be written as

$$H(t) = A(\frac{t}{t_f}) \sum_{i}^{n} h_i \sigma_i^x + B(\frac{t}{t_f}) H_{\text{spin}}, \quad (8)$$

where $A(\frac{t}{t_f})$ smoothly evolves from 1 to 0 and $B(\frac{t}{t_f})$ goes reversely.

However, AQC cannot be achieved easily for the following reasons: (i) one need to find gap_{min} of the problem Hamiltonian for ensuring an adiabatic evolution, which is equivalent to find the ground state of it; (ii) even if the evolution of time can be given in advance, decoherence and noise can affect the performance of the algorithm massively. Thus, quantum annealing accelerate the evolution by tunneling the traverse magnetic faster, which reduces the computing time. The quantum system can be excited to a higher energy state during the process, but still remains a relative high possibility of obtaining a ground state of the problem Hamiltonian once the initial traverse magnetic is switched off. Following this idea, quantum annealer as computing platform has been built by concluding the global minimum with statistical methods.

IV. EXPERIMENTS

A. HiQ simulator

38 qubits

B. IBM/Rigetti cloud quantum conputer

to be decided by Kike

C. Quantum annealer simulator

stoquastic Hamiltonian, doable

D. D-Wave quantum annealer

D-Wave 2000Q

V. DISCUSSION

comparison with DP

Potential enhancements

VI. CONCLUSION

to be written at the end

VII. ACKNOWLEDGMENTS

We acknowledge funding from projects QMiCS (820505) and OpenSuperQ (820363) of the EU Flagship on Quantum Technologies, Spanish Government PGC2018-095113-B-I00 (MCIU/AEI/FEDER, UE), Basque Government IT986-16, Shanghai Municipal Science and Technology Commission (18010500400 and 18ZR1415500), and the Shanghai Program for Eastern Scholar, as well as the and EU FET Open Grant Quromorphic. This work is supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR) quantum algorithm teams program, under field work proposal number ERKJ333.

[1] cite something