Logistic Network Design with a D-Wave Quantum Annealer

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(Dated: June 25, 2019)

Logistic network design is an abstract optimization problem which, under the assumption of minimal cost, determines the optimal configuration of infrastructures and facilities of the supply chain based on customer demand. With the solutions at hand, key economic decisions are taken about the location, number, as well as size of manufacturing facilities and warehouses. Therefore, an efficient method to address this question, which is known to be NP-hard, has relevant financial consequences. Here, we propose a hybrid classical-quantum annealing algorithm to accurately obtain the optimal solution. The cost function with constraints is translated to a spin Hamiltonian, whose ground state is supposed to encode the searched result. This algorithm is realized on a D-Wave quantum computer and positively compared with the results of the best classical optimization algorithms. This work shows that state-of-the-art quantum annealers may address useful chain supply problems.

I. INTRODUCTION

Calculating the global minimum (maximum) of a multi-variable function could be arduous, especially when the number of variables and constraint conditions grow and the objective function is highly non-linear, the problem is NP-hard. It is even too complicated to verify whether a given solution is the optimal one or not. As a branch of optimization problem, logistic network design problem (NDP), covers a huge set of decision making problems for management issue [1], e.g. where to place facilities and how to assign customers minimizing the total cost, or how to redistribute driving paths of vehicles to reduce traffic jams. Several classical algorithms are proposed for optimization problems, from the very beginning mathematical analysis for small scales, e.g. branch and bound, context partition and dynamical programming, then metaheuristic algorithm based on single solution such as hill climbing, simulated annealing [2], and tabu search [3, 4], to intelligent optimization by genetic algorithm [5], ant colony optimization [6, 7] and the artificial neural network [8]. This algorithm has been applied to study NDP and provided some preliminary results [9–12]. However, the mathematical principles of these algorithms for finding global minima are not systematically established and, in most cases, it requires experience adjusting parameters. This arises the demand on developing an interpretable algorithm for solving NDPs efficiently.

In this Article, we address the aforementioned problem by employing quantum annealing [13, 14], which theoretically accelerates the annealing process due to quantum tunneling. Making use of a small annealing time in comparison with any classical algorithm, the ground state of the effective Hamiltonian is generated and decoded to achieve the optimal solution with respect to the objective function [15]. Current D-Wave cloud quantum annealer comprises 2048 qubits distributed in a hardware architecture according to the Chimera graph. The constraints imposed by the architecture generally allow for solving only relatively small problems, which can be enhanced when combined with classical algorithms. Additionally, in practice, the quantum device is affected by thermal fluctuations, decoherence, and I/O errors, which prolong the computation time because of extra error-correction process and decrease the accuracy of the solutions. However, quantum annealers have proven their capability to deal with hard problems in different fields, such as condensed matter physics [16–20], engineering [21], cryptography [22, 23], biology [24] and finance [25–27], among others. This shows that current technology is ready to realize quantum annealing algorithm under certain circumstances. More specifically, solving NDP using quantum annealing requires classical feedback from specific qubits during the annealing process, a feature which is not currently supported by D-Wave. Inspired in Ref. [28], we propose an alternative approach, called combined quantum annealing algorithm, which makes use of two layers with feedback-control interaction between them. The approach is tested by 12 NDPs employing both the simulator and the D-Wave cloud quantum annealer, achieving remarkable results when compared with the classical ones. This supports the extended idea that hybrid quantum-classical algorithm will allow us to enlarge the solvable problems with quantum computers, accelerating the development of quantum technologies.

This manuscript is organized as follows: in Sec. II, we formulate NDP as a constrained 0 – 1 programming problem, which will afterwards allow us to map it into the Chimera architecture. In Sec. III, we introduce the fundamentals of quantum annealing and of the combined quantum annealing algorithm. Afterwards, in Sec. IV, we experimentally tests the optimization of NDPs by comparing the results against the best known classical ones,

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as well as those given by a classical algorithm for finding global minimum. Finally, in Sec. V, the results are analyzed and possible alternative software and hardware approaches for further enhancement are discussed. The conclusions of this work are listed in Sec. VI.

II. MODEL

Although logistic network design problem could be described in an abstract framework, we choose the customer-facility picture to model it, before we introduce the combined quantum annealing algorithm. Suppose that there are at most \( m \) sites for potential facilities and \( n \) customers to be allocated. The indices \( J = \{1, 2, \cdots, m\} \) and \( I = \{1, 2, \cdots, n\} \) denotes the set of potential location sites and the set of customers, respectively. It costs \( f_j \) to build a facility with capacity of \( v_j \) placed at site \( j \in J \). When a customer \( i \in I \) with demand \( d_i \) is served by facility \( j \), the transportation process brings \( c_{ij} \) to the cost. One has to find the way to allocate customers with minimum total cost that ensures all customers are served and none of the facilities is overflowed. To formulate the model, one has to minimize the following cost function

\[
\text{cost}(x_j, y_{ij}) = \sum_j f_j x_j + \sum_i \sum_j c_{ij} y_{ij},
\]

where \( x_j \) and \( y_{ij} \) are binary variables that represent the allocation configuration. A facility is built at site \( j \) when \( x_j = 1 \), where customers could be only served in the sites with facilities. Accordingly, \( y_{ij} = 1 \) means customer \( i \) is assigned to facility in site \( j \), where other facilities are no longer available for this customer. These constraint conditions can be written as

\[
\sum_j y_{ij} = 1, \forall i \in I,
\]

\[
\sum_i d_i y_{ij} < v_j, \forall j \in J,
\]

\[
y_{ij} \leq x_j, \forall i \in I, \forall j \in J.
\]

Minimizing this model is proven to be an NP-hard problem, i.e. obtaining its global minimum value highly time-consuming. It is also inefficient to verify if a given network is the solution that minimize the cost function. These features lead to the demand on specific algorithm that accelerate the searching process and enhance the quality of solution.

III. COMBINED QUANTUM ANNEALING ALGORITHM

Quantum annealing ideally allows us to slowly modify a parameter in its Hamiltonian keeping the system in the ground state. For example, in a spin-1/2 Hamiltonian annealer, the total Hamiltonian is split into a tunneling Hamiltonian and a problem Hamiltonian codifying the solution for the problem,

\[
H = \left(1 - \frac{t}{t_f}\right) \sum_i \hat{s}_i^2 + \frac{t}{t_f} \left(\sum_i h_i \hat{\sigma}_i^z + \sum_{i>j} J_{ij} \hat{\sigma}_i^+ \hat{\sigma}_j^-\right).
\]

The system is supposed to be in the ground state of the problem Hamiltonian when \( t = t_f \). If we introduce the qubit operator \( \hat{x} \) with eigenvalues 0 and 1, such that \( \hat{x}(0) = 0 \) and \( \hat{x}(1) = 1 \), respectively, quadratic unconstrained binary optimization (QUBO) problem can be mapped to a spin-1/2 quantum annealing problem by \( \hat{x} = (1 + \hat{\sigma}_z)/2 \).

Looking at the cost function given by Eq. (1), one notices that it cannot be directly optimized by quantum annealing, since there are constraints. Although an effective QUBO Hamiltonian may be constructed satisfying Eq. (2) and Eq. (3), the constraint given by Eq. (4), which imposes that customers to be served in correct sites, can not be satisfied during the quantum annealing process. This requires extracting information from qubits representing facility locations and perform feedback during the annealing process for controlling and dynamically tuning the size of the Hamiltonian, a feature which is not currently available. Thus, quantum annealing should be combined with a classical algorithm to obtain the global minimum. Inspired by Ref. [28], we apply here a combined quantum annealing algorithm comprising two layers, namely, the outer layer in which the optimization for facilities’ locations is performed by a simulated annealing algorithm, and the inner layer, in which the quantum annealing process runs.

In the outer layer, a list with elements \( x_j \), sorted by index \( j \) in ascending order, denotes the neighboring configuration of facilities, while a neighboring function operates on the list to generate a new configuration in three ways: (i) pick a \( x_j \) with value 1, and set it to 0, which means a facility is randomly closed; (ii) pick a \( x_j \) with value 0, and set it to 1, which means a facility is randomly built on a site; (iii) swap the values of \( x_j \) and \( x_k \), if their values are different, which means a facility moves to another site. A dice will be thrown to decide which operation is carried out by the neighboring function on the list, while all the operations should be allowed, e.g. when all facilities are open, operation (ii) is no longer available.

In the inner layer, we perform quantum annealing to minimize \( \sum_i \sum_j c_{ij} y_{ij} \) under constraint given by Eq. (2), Eq. (3), and Eq. (4). As we mentioned before, the latest quantum annealer is designed to solve QUBO problems, i.e. to minimize the objective function \( \text{obj}(\mathbf{x}) = \mathbf{x}^T \mathbf{Q} \mathbf{x} \), that \( \mathbf{Q} \) is the QUBO matrix and \( \mathbf{x} \) is the binary vector. We map binary variables \( y_{ij} \) to qubit \( q_{(i,j)} \), and allowed \( j \) are the sites on which facilities are built. To introduce the constraint given by Eq. (2), we construct weighted penalty functions to formulate an effective unconstrained
Hamiltonian, e.g. $\lambda_i(\sum_j q_{(i,j)} - 1)^2$, for customer $i$ to guarantee that customer $i$ is associated only to one facility, with a reasonable $\lambda_i$. Accordingly, Eq. (3) may also be written as $\mu_j(\sum_i d_i q_{(i,j)} + (2, a_j) - v_j)^2$ for facility $j$, with slack variables encoded by ancilla qubits. Here, $(2, a_j)$ denotes the binary expansion $\sum_{i=0}^k 2^i a_{(i,j)}$ which implies that the number of ancilla qubits to required to introduce the constraint is $k = \lceil \log_2 v_j \rceil$. The problem Hamiltonian is hence given by

$$H_p = \sum_i \sum_j c_{ij} q_{(i,j)} + \sum_i \lambda_i \left( \sum_j q_{(i,j)} - 1 \right)^2 + \sum_j \mu_j \left( \sum_i d_i q_{(i,j)} + (2, a_j) - v_j \right)^2,$$

which could be mapped to a solvable spin-1/2 Hamiltonian for the annealer. The ground state of the problem Hamiltonian is supposed to be the configuration that minimize the classical objective function with reasonable penalty strength $\lambda_i$ and $\mu_j$.

This combined quantum annealing algorithm works as follows: (i) Set the optimal solution to infinity and generate an initial configuration as the optimal configuration of facilities. Schedule the annealing process, i.e., the cooling rate, initial temperature, final temperature, etc. (ii) Flip the values of variables $x_j$ in list by neighboring function and obtain a new configuration $\tilde{x}_j$. (iii) Quantum annealing according to the neighbour configuration, decode the state of qubits to $\tilde{y}_{ij}$ and calculate value of the cost function $\text{cost}(\tilde{x}_j, \tilde{y}_{ij})$. (iv) Apply the Metropolis algorithm that if $\text{cost}(x_j, y_{ij}) > \text{cost}(\tilde{x}_j, \tilde{y}_{ij})$, we accept the new configuration and value as the optimal ones and go for next step. Otherwise, randomize $\rho \in (0, 1)$, if $\rho < \exp(-(\text{cost}(\tilde{x}_j, \tilde{y}_{ij}) - \text{cost}(x_j, y_{ij}))/T)$, we also accept them and continue. We go for the next step without operations if new configuration and value are denied. (v) Increase the iteration index by one and check if it meets the upper limit. Once it is larger than the maximum iteration number, we adjust the annealing temperature according to the schedule, reset the iteration index and go for the next step. Otherwise, return step (ii). (vi) Output the optimal solution if the current temperature is not higher than the target temperature. Otherwise, return step (ii).

Thus, if all parameters in the outer and inner layers are correct and the quantum annealer is noiseless, the sites for building facilities, the allocation of customers and the optimized total cost should be obtained by this combined annealing algorithm. Additionally, error correction could be applied to provide a quasi-optimal solution, which is a relevant advantage when employing a noisy and incoherent quantum annealer.

IV. EXPERIMENTS

We choose the same twelve problems tested by Ref. [28], which are open-source NDP test problems from OR-Library [29]. The optimal solution is given by the author using Lindo software. We encoded the logical qubits by $q_{(i,j)}$ and ancilla qubits by $a_{(i,j)}$. The connectivity of these qubits are connected intensively, that the number of couplers is estimated by

$$\text{len}(\text{coupler}) = \frac{(m-1)mn}{2} + \frac{(n-1)nm}{2} + \frac{(k-1)kn}{2} + nkm,$$

where each term is contributed by the couplers between logical qubits because of Eq. (2), Eq. (3), couplers between ancilla qubits and couplers that link an ancilla qubit to a logical qubit (see Fig. 1). To solve a NDP problem with $m$ sites for potential facilities and $n$ customers to be allocated, we need at least $n \times m + k \times m$ qubits to implement the effective Hamiltonian on a quantum annealer. Notice that this number can be much higher for a minor embedding, considering that the topology of the device is different from the connectivity graph of the problem. The smallest problem for testing requires 1056 qubits with 40320 couplers, which cannot be directly implemented on a 2048-qubit D-Wave quantum annealer because of its limited connectivity (6016 couplers). An open-source software qbsolve developed by D-Wave [30] could split a large QUBO problem to sub-problems which are available for embedding, while the sub-problems are solved by local simulator with tabu al-
algorithm or a real quantum annealer under authorized license. To solve a problem with a D-Wave quantum annealer, the submission of a QUBO or Ising problem will be sent to a server for queueing. The result will be retrieved from the cloud platform once the annealing is performed. Although the computing time in a real annealer is negligible, one trial of solving a large QUBO matrix could be very time-consuming (about 15 minutes for a 900 × 900 QUBO matrix), since it requires solving many sub-problems partitioned in the main loop of qbsolv. The network transmission and queueing is highly time consuming, making impossible to solve the problem by a cloud quantum annealer. So we choose to solve the problem by a local simulator provided by D-Wave, and refine the result by D-Wave 2000 after obtaining the configuration of facilities.

The initial temperature of simulated annealing is set to be 10000, which is scaled to a reasonable value considering the deviation between the new and old value of cost function. For simplicity, we choose α = 0.5 as cooling rate and the schedule as scale cooling. The maximum iteration number is m and the target temperature is 1. To obtain the optimal solution according to a given configuration of facilities, the penalty strength should be strong enough, i.e., it should ensure that the problem Hamiltonian’s ground state satisfies all constraint conditions. Hence, if the quantum annealer is noiseless, the parameters could follow λ_j ≫ µ_i ≫ c_{ij}, which promise that a customer is assigned to only one facility, none of the facility is overflowed, and the configuration refers to a minimal total cost. However, in practice, quantum device is affected by thermal fluctuation or inaccuracy of magnetic field tunneling that the result is chaotic which only satisfies constraint conditions but far from optimal solution. Thus, the penalty strength is set to be slightly larger than c_{ij} for the possibility of obtaining an optimal solution. Although this sometimes breach constraint conditions because of the device noise, such violation could be corrected by repeat the quantum annealing process until all constraint conditions are satisfied. After studying the dataset, the penalty strength λ_i are set to be min_j(c_{ij}), while µ_i are almost negligible considering the demands and capacities.

The results are presented in Table I, while the detailed parameters for simulated annealing algorithm are given in Ref. [28]. Considering m sites for potential facilities and n customers to be allocated, the total number of iterations of the simulated annealing algorithm is 5nm × [log_{0.95} 0.01] = 450nm, and the according combined quantum annealing algorithm takes only m × [log_{0.0001} 5] = 14m runs for Metropolis acceptance criterion. The data of the combined quantum annealing algorithm are taken from several results fluctuating within a small range without preference. We also demonstrate how the algorithm works for Problem cap71 depicting its crucial intermediate steps in Fig. 2(a) and Fig. 2(b).

| Problem | Size | Lindo | SA | QA |
|---------|------|-------|----|----|
| cap71  | 16 × 50 | 932615.7500 | 1192413.575 | 934544.7125 |
| cap72  | 16 × 50 | 977799.4000 | 1012970.190 | 983484.8250 |
| cap73  | 16 × 50 | 1010641.4500 | 1100470.190 | 1012476.975 |
| cap74  | 16 × 50 | 1034976.9750 | 1212970.190 | 1034976.975 |
| cap101 | 25 × 50 | 796648.4400 | 886494.4750 | 797257.3500 |
| cap102 | 25 × 50 | 854704.2000 | 998953.6250 | 855668.3000 |
| cap103 | 25 × 50 | 893782.1125 | 102291.150 | 895309.9125 |
| cap104 | 25 × 50 | 928941.7500 | 1177291.150 | 928941.7500 |
| cap131 | 50 × 50 | 793439.5620 | 856571.4500 | 799725.4625 |
| cap132 | 50 × 50 | 851495.3250 | 1011571.450 | 851753.5875 |
| cap133 | 50 × 50 | 893076.7120 | 1219071.450 | 893226.1625 |
| cap134 | 50 × 50 | 928941.7500 | 1374071.450 | 929477.5625 |

TABLE I. The combined quantum annealing algorithm is tested by 12 NDP problems from OR-Library while the results are listed under QA. The optimal solutions are compared with the best result from Lindo given by the author of Ref. [28] and classical simulated annealing algorithm denoted by SA.

V. DISCUSSION

Before any further discussion on enhancing its performance, let us analyze the experimental results for a better understanding of the protocol. At this moment, we sacrifice the cloud D-Wave quantum annealer in the test problems from Table I for the sake of saving QPU resources and total computation time. One may estimate that solving the problem without a local solver takes about 56 hours for a relative small problem cap71 and the QPU time every month is very limited. Even though the result provided by a local simulator is sufficiently accurate, with a maximal deviation upper bounded by 0.5%, it could be straightforwardly reduced by repeating the inner layer several times to search for better solutions. We also notice that, normally, the local simulator does not provide an optimal solution (or very close solution) the first time for any configuration of facilities, but the solution improves by solving the same problem once the according input is generated by the neighboring function again. As we mentioned before, we could refine the result after obtaining the optimal configuration of facilities by D-Wave 2000 to save QPU time, while verifying the reliability of D-Wave 2000. We choose again Problem cap71 and generate the QUBO problem with the configuration of facilities given by the simulator for the cloud quantum annealer. As shown in Fig. 2(b) and 2(c), the noise of the device is acceptable comparing to an ideal simulator, and one can straightforwardly improve the results employing several refinements. The search space by exhaustive searching for a QUBO matrix encoded by n × m logical qubits and k × n ancilla qubits is 2^{(n+k)m}, and the search subspace is reduced massively once the quantum annealer excludes most of the states with higher energy than those low-energy states. Then, we point out that this algorithm still works even if the quantum annealer (simulator or real device) in the inner layer is noisy and
FIG. 2. (a) The initial configuration of facilities and its status before each cooling. Each column is a list vector that represents the sites from up to down, where a green or red block denotes a facility is built here or not. (b) The evolution of best solution before each cooling and the refining process are shown by blue dashed line and red solid line, respectively. In these experiments, the optimal total costs result in 932739.0875 and 932946.3250, which are better than the one in Table I. (c) The allocation of customers of the best result in 932739.0875 and 932946.3250, which are better than respectively. In these experiments, the optimal total costs result in 932739.0875 and 932946.3250, which are better than the one in Table. I. (c) The allocation of customers of the best solution after refinements.

Incoherent, but that it takes more redundant refinement process in the inner layer algorithm, i.e. to apply quantum annealing for many times in the inner layer and keep the best solution that satisfies all constraint conditions.

Now we propose several approaches to make the algorithm more efficient. From the perspective of algorithm, the outer layer applies a classical simulated annealing algorithm which theoretically obtains global minimum with adequate annealing parameters. As we mentioned before, the inappropriate annealing schedule will stuck the algorithm to a local minimum and we should find the initial temperature for simulated annealing. The total iteration number to guarantee a global minimum is enormous which is proved by Ref. [31], while the transition probability from state $i$ to state $j$ is denoted by $P_{ij} = G_{ij}A_{ij}$. The acceptance probability follows the Metropolis acceptance criterion that $A_{ij} = \exp(-(E_j - E_i)/T)$ when $E_j > E_i$, otherwise $A_{ij} = 1$. We assume that the generation probability is symmetric $G_{ij} = G_{ji}$ and the Markov chain of a given temperature is acyclic and irreducible, then the system follows a Maxwell-Boltzmann distribution that

$$
\pi_i = \frac{|N(i)| \exp(-E_i/T)}{\sum_j |N(j)| \exp(-E_j/T)},
$$

where $N(i)$ and $N(j)$ denote the sets of neighbours of state $i$ and $j$, respectively, and generation probability $P_{ij}$ is distributed uniformly among neighbours of state $i$ (i.e., $G_{ij} = 1/|N(i)|$ if $j \in N(i)$). Accordingly, the acceptance probability $\chi(T)$ and an iteration algorithm to obtain the proper annealing schedule are provided and proved in Ref. [32]. In this way, we could analyze the dataset and find optimal parameters for the outer layer algorithm before solving the NDP problem with combined quantum annealing algorithm. In the inner layer, quantum annealing for a large QUBO matrix cannot be implemented directly which requires qbsolv for generating subproblems. However, the partition algorithm in the main loop of qbsolv sometimes leads to local minimum that requires better method for splitting the matrix. An alternative algorithm could be introduced, e.g., embedding larger subproblems that exploiting the resource of the quantum annealer [33]. Meanwhile, the quantum annealing algorithm in the inner layer is affected by the penalty strength, while these parameters are very tricky to be decided. One should scale them according to the dataset and the noise of the hardware, for obtaining an acceptable solution that satisfies all constraint conditions. We notice that the optimized penalty strength for a QUBO problem could be given with the combination of machine learning algorithm, e.g., gradient descent as the most trivial idea, by quantum annealing with variant parameter vectors $\lambda$ and $\mu$ and stop at an optimal solution.

On the hardware side, the priority is to own a D-Wave quantum annealer instead of using cloud quantum annealer, considering that the inner annealing time does not contribute a lot to the whole computation time. An advance could be controlling the quantum annealing process in the inner layer. Generally, the Hamiltonian of a quantum annealer $H = A(t)H_T + B(t)H_P$ is constrained by boundary conditions that $A(0) = 1, A(t_f) = 0, B(0) = 0$ and $B(t_f) = 1$, to start with an initial tunneling Hamiltonian and result in the ground state (or low-energy state) of the final problem Hamiltonian. A customized quantum annealing process might shorten the annealing time while reduce the excitation to generate a better solution within less time. This annealing protocol could be given by control theory or other optimal methods, e.g., shortcut to adiabaticity in spin system [34–37], that controls the preparation and evolution of qubits in the quantum annealer. Quality of the solutions could also be improved by quantum annealer with more qubits, larger connectivity and less noise, which will be released by D-Wave in mid-2020 named Pegasus [38]. An alternative hardware will be coherent quantum annealer which is still far from practical application but could be built with current technologies while providing preliminary results [39–41].

VI. CONCLUSION

We proposed a combined quantum annealing algorithm inspired in Ref. [28] to solve logistic network design problems, but which can also be applied to a large variety of optimization problems. The algorithm is implemented in a local simulator and, partially, in a D-Wave quantum an-
nealer. Then, the implementation is tested with 12 NDP problems and the results are in very good agreement with the already-known best solutions given by *Lindo*. This research is another convincing evidence for the feasibility of applying quantum annealing for optimization problems, even when the quantum devices are limited by the number of qubits, the connectivity, and the noise.

**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.

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