

Community Detection Across Emerging Quantum Architectures

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Abstract—One of the roadmap plans for quantum computers is an integration within HPC ecosystems assigning them a role of accelerators for a variety of computationally hard tasks. However, in the near term, quantum hardware will be in a constant state of change. Heading towards solving real-world problems, we advocate development of portable, architecture-agnostic hybrid quantum-classical frameworks and demonstrate one for the community detection problem evaluated using quantum annealing and gate-based universal quantum computation paradigms.



1 INTRODUCTION

During the last two years a race of industrial and research organizations has been opened to develop a ready-to-implement engineering solution for quantum computing (QC). It resulted in the QC market closely resembling the ascent ages of classical computing industry. Namely, there were many underdeveloped computing architectures which being incompatible with each other required significant efforts in porting software and algorithmic solutions between them. Given a broadly supported opinion that in the near term we are unlikely to become witnesses to flexible large-scale quantum architectures, there is a critical need to develop portable, architecture-agnostic hybrid quantum-classical frameworks that will allow solving large-scale computational problems on small-scale quantum architectures.

There are multiple emerging quantum computation paradigms. The performance comparison of these paradigms is an important research topic. In this paper, we present for the first time a performance comparison of two leading quantum computation paradigms - D-Wave quantum annealing and gate-based universal quantum computation. Both approaches have great potential for achieving quantum speedup for a number of important problems [1], [7], [13], [27].

The first approach, quantum annealing (QA), is based on adiabatic quantum computation (AQC) [17]. QA solves computational problems by using a guided quantum evolution [32]. The evolution starts with an initial Hamiltonian with an easy-to-prepare ground state and ends up in the ground state of the problem Hamiltonian. QA is based on the adiabatic theorem that guarantees that if the Hamiltonian is evolved slowly then transitions to excited states are suppressed during the adiabatic evolution [32]. The D-Wave quantum annealer uses superconducting flux qubits [2], [6] and has been shown to solve optimization problems on graphs [31], machine learning [22], traffic flow optimization [18], and simulation problems [12]. Quantum and hybrid quantum-classical approaches have been employed.

The second approach is often referred to as the gate-based or universal QC. This mode of QC was theoretically demonstrated to have a great potential for exponential speedups over best known classical algorithms [21]. In the near term, the capability of the quantum devices is limited by the number of qubits, low fidelity of gates, and lack of error correction. These limitations constrain us to using low-depth quantum circuits (i.e., quantum circuits with few gates) on a small number of qubits. Within the constraints of near-term intermediate-scale quantum (NISQ) technology [26], a number of hybrid quantum-classical algorithms were developed and experimentally demonstrated to solve small problems. One of the most promising of such algorithms is Quantum Approximate Optimization Algorithm (QAOA) [8], [9]. QAOA is inspired by adiabatic quantum computation. Similarly to AQC and QA, the evolution path starts with an easy-to-prepare Hamiltonian in the ground state and evolves to the final Hamiltonian that encodes the solution of the problem remaining in the ground state. However, unlike QA in QAOA the evolution is performed by applying a series of parametrized gates called ansatz [16] which is parametrized by a set of variational parameters. This is accomplished by a hybrid approach that combines quantum evolution and classical variational optimization for optimal QAOA parameters [32] with the goal of finding the evolution path that prepares the ground state of the problem Hamiltonian.

2 METHODOLOGY

This work addresses three main challenges. First, we show how to use quantum computing to solve the community detection problem, a well known NP-hard problem. Second, we present an approach to solving realistic large problems using the NISQ hardware with a limited number of noisy qubits. Third, we demonstrate a method that is portable across two leading quantum computation paradigms and can be easily extended to future hardware.

The community detection problem (or modularity graph clustering) has a variety of applications ranging from biology to social network analysis [3], [20], [25], [30]. Its complexity [4] and practical importance justify an attempt to solve it using QC. The goal of the community detection is to split nodes of a graph $G = (V, E)$ into communities by maximizing its modularity [19]:

$$H = \frac{1}{4|E|} \sum_{ij} (A_{ij} - \frac{k_i k_j}{2|E|}) s_i s_j = \frac{1}{4|E|} \sum_{ij} B_{ij} s_i s_j, \quad (1)$$

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where $s_i \in \{-1, +1\}$ are variables indicating node i th community assignment, k_i is a degree $i \in V$, and A is the adjacency matrix of G . In this paper, we will focus on clustering the graph into two communities. There are several approaches to generalize the problem for cases when the number of communities is greater than 2.

The clustering of large networks is currently impossible with existing quantum computers because of the small number of available qubits. This limitation applies both to quantum annealing [31] and universal quantum computing [24]. To tackle large problems using available quantum hardware, we use a hybrid quantum-classical local-search approach. Our approach is inspired by existing numerous local-search heuristics (see [28] for a review). Our algorithm finds a solution to the global community detection problem by selecting subproblems small enough to fit on the target quantum computer, solving them using a quantum algorithm and iterating until the solution to the global problem is found. The outline is presented in Algorithm 1.

Algorithm 1 Community Detection

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procedure COMMUNITY DETECTION(Graph  $G$ )
  solution = initial_guess( $G$ )
  while not converged do
     $X$  = populate_subset( $G$ )
    // using QAOA or D-Wave QA
    candidate = solve_subproblem( $G, X$ )
    if candidate > solution then
      solution = candidate

```

In particular, we start with a random community assignment. At each step we select a subproblem (subset of vertices $X \subset V$) by taking the vertices with highest potential gain if moving them from one community to another. The gain for each vertex can be computed efficiently [19]. Then we fix the community assignment of all $i \notin X$, encode them into the problem as boundary conditions (denoted by \tilde{s}_j , a typical technique in many heuristics [11], [15]) and maximize

$$\begin{aligned}
 Q_s &= \sum_{i>j} \sum_{i,j \in X} 2B_{ij}s_i s_j + \sum_{i \in X} \sum_{j \notin X} 2B_{ij}s_i \tilde{s}_j \\
 &= \sum_{i>j} \sum_{i,j \in X} 2B_{ij}s_i s_j + \sum_{i \in X} C_i s_i.
 \end{aligned} \quad (2)$$

The subproblems are solved using QC. To satisfy the constraints of available hardware, we fix the subproblem size to some small number (in our experiments, it was 25).

3 IMPLEMENTATION DETAILS AND RESULTS

We implement our local search algorithm in Python using the graph methods provided by NetworkX [10]. The novelty of our approach is that it allows to use D-Wave QA, QAOA and classical Gurobi [23] solvers interchangeably simply by passing different flags, enabling rapid prototyping and direct comparison of different methods as the hardware and its capabilities evolve. Additionally, Gurobi was used as a global optimization solver for the sake of quality comparison. To our knowledge this is the first attempt to directly compare universal quantum computing and quantum annealing. Our framework is also easily extendable, making it possible for researchers to add new backends as they become available. We plan to release the framework as an open-source project.

Our results are presented in Figure 1. In these experiments, we used the Intel-QS [29] simulator for QAOA (at the time our group did not have access to a universal quantum computer of sufficient size). We use six real-world networks from the

KONECT dataset [14] with up to 400 nodes as our benchmark. For each network, we ran 30 experiments with different random seeds. The same set of seeds is used between three backend solvers, making the results directly comparable. The subproblem size is fixed at 25 (i.e., 25 qubits are used). Our results demonstrate that the quantum local search approach with both quantum methods is capable of achieving results comparable to state-of-the-art, with a potential to outperform as hardware evolves.

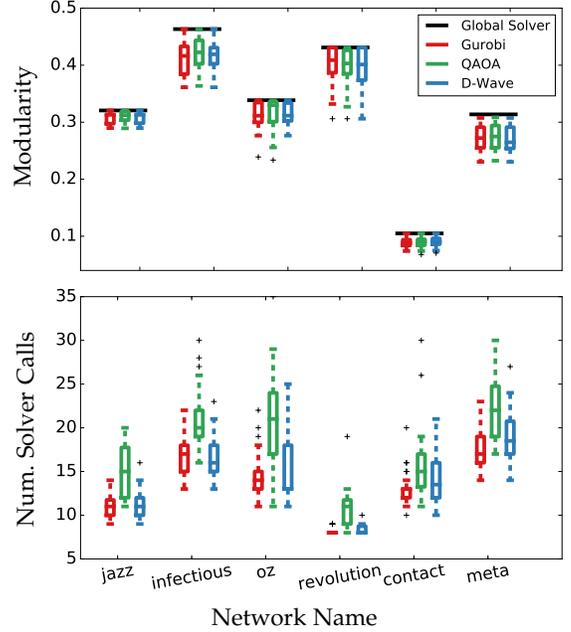


Fig. 1. Box-plots comparing modularity scores (greater is better) and number of solver calls (less is better) respectively for the three different solvers. For the graph oz , Gurobi and D-Wave returned a modularity score greater than the Global Solver (best known value)

4 DISCUSSION

In the near term, quantum hardware will be in a constant state of change. Many different NISQ-era hardware solutions will appear and some will be abandoned. In the midst of such evolutionary times, we want to be able to continue research in quantum algorithms and head towards solving real-world problems. To accomplish this, we need portable, architecture-agnostic hybrid quantum-classical frameworks that will allow solving large-scale computational problems on small-scale quantum architectures. Moreover, these frameworks need to be robust and future-proof. In this work, we have presented a prototype of such a framework for solving the problem of community detection in networks on two distinctively different architectures: D-Wave quantum annealer and universal quantum computer. We suggest extending this approach for solving other types of problems in science.

The constant change of hardware and overall immaturity of the existing technology leads to many risks in QC. In spite of major effort, it has not been experimentally demonstrated yet an ability to achieve speedups over state-of-the-art classical supercomputers and there are valid concerns about scalability of existing implementations [5]. Advances in material design and engineering will allow the community to overcome those hurdles. We expect QC to eventually become a part of the HPC ecosystem with an initial role as an accelerator providing a new layer of parallelism. Our approach will provide for co-design exploration towards the best QC accelerator choice for an application mix.

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