Seminar: Advanced Topics in Quantum Computing On efficient encodings for QAOA solutions to vehicle routing problems

Eben Jowie Haezer October 18, 2023

Abstract

This report details recent advances in the optimisation of computing resources for quantum approaches to solving the vehicle routing problem (VRP) and its variants. This set of problems is of significant importance with regard to logistical applications in industry. In accordance with the input constraints of the quantum hardware, the problem is formulated as a quadratic unconstrained binary optimisation (QUBO). A simple approach known as the full encoding results in each solution represented by a unique basis state, thereby requiring one qubit per classical variable. Due to this inefficiency in resource allocation when considering the at worst factorial search space, a more optimised minimal encoding is suggested that offers a logarithmic reduction in necessary computing power. In spite of certain drawbacks incurred by employing this minimal encoding, experiments have shown that the solution quality is not heavily impacted.

I. Introduction

The Vehicle Routing Problem (VRP) is concerned with finding optimal routes for vehicles to deliver goods to a set of customers with some geographical distance between them. It is obvious that this type of problem has far reaching practical applications in various contexts, in fact the need to find a reasonable solution is almost ubiquitous when dealing with logistical planning, for example to determine efficient road, rail, shipping, and air routes for commercial or public interest.

VRP, being itself a more general version of the Travelling Salesman Problem (TSP), is similarly an NP hard combinatorial optimisation problem with a solution space scaling factorially in the number of customers, and thus finding the definitive optimal solution already becomes intractable at two digit customer counts. The most optimal classical algorithms known to date and used in practice employ heuristics and greedy methods to construct routes within single digit percentage tolerances.

More recently, the noisy intermediate scale quantum (NISQ) era has paved the way for the development of variational quantum algorithms alongside the potent quantum annealing method as a contender for computing reliable and near optimal solutions to combinatorial optimisation problems, exploiting the unique inherent property of

quantum algorithms to operate on the entire solution space at once, albeit incrementally and probabilistically.

Initial tests have shown some promise in applying these quantum algorithms to the VRP against classical solvers, achieving comparable accuracy on small problem instances. As quantum hardware continues to improve, it makes sense to also look at utilising it as efficiently as possible. Solving VRP naively using quantum methods maps one classical variable to one whole qubit, quickly exhausting the already limited computing resources when introducing additional constraints such as vehicle capacity or time windows on larger problem scales more commonly encountered in practical scenarios.

This report discusses recent research into an idea to mitigate this uneconomical use of computing power through a more clever and refined encoding of the input problem, in order to achieve a logarithmic correlation between problem size and resource consumption. Section II outlines a formal description of the VRP and some of its variants. Section III explains the QUBO and its application to solving the VRP on quantum hardware, along with a brief mention of the closely related Ising model and in particular its Hamiltonian function. Section IV details the encoding approaches onto the quantum system and lists benefits and drawbacks for each. Published experimental observations de-

scribing the impact of the encodings are discussed in Section V, and the report concludes in Section VI.

II. Vehicle Routing Problem

The vehicle routing problem (VRP) is a generalisation of the perhaps more well known NP hard Travelling Salesman Problem (TSP). VRP seeks the optimal route or routes for a number of vehicles to traverse in order to deliver certain goods to customers in various locations.

The problem is modelled intuitively by a graph G=(V,E) where each node or vertex $v_i \in V$ represents the location of a customer and each edge $(i,j) \in E$ connecting two vertices corresponds to a path traversible by a delivery vehicle. $\|V\|=N$ is then the number of customers considered. Traversing an edge (i,j) typically incurs a cost represented by $c_{ij} \in \mathbb{R}_{\geq 0}$, of which the total value summed up across the entire journey is to be optimised, ie. made as small as possible. This cost may be set based on travel time, distance, or other concerns with economic consequences.

Vehicles may only travel across edges. Furthermore, each graph contains a designated node $v_0 \in V$ known as the depot. Valid routes must always begin and end at the depot. A valid route is then a tuple $(v_n, v_{n+1}, ..., v_m)$ s.t. $v_n = v_m = v_0 \wedge \forall n. \ (v_n, v_{n+1}) \in E$.

For a problem to be classified as VRP, it should fulfil at least the above minimal constraints. However, additional constraints may be imposed as needed to better reflect a practical use case at the expense of slightly complicating the model. For example, the capacitated VRP or CVRP stipulates a fixed upper bound on the carrying capacity of each vehicle leaving the depot, where in most cases this value is consistent across all vehicles. Customers v_i are then assigned a score $d_i \in \mathbb{R}_{\geq 0}$ reflecting their demand quantity. This introduces the complication of optimising for capacity and demand as well as edge cost, and the ideal solution for a given graph will most likely differ from the simple VRP.

On the other hand, the VRP with time windows (VRPTW) introduces a secondary time parameter. Customers v_i are assigned a certain time window $[t_i^0, t_i^f] \subseteq \mathbb{R}_{\geq 0}$ in which they expect a delivery. For the depot v_0 this interval is $[0, \infty)$ for simplicity. Hence the edge costs c_{ij} represent travel time between two nodes in this formulation, and the objective shifts to finding the optimal route that serves all customers whilst respecting these time windows, or failing this attempting to maximise the number of customers or total goods supplied.

III. Problem Formulation

The quadratic unconstrained binary optimisation (QUBO) is concerned with finding a binary vector $|x^*\rangle \in \{0,1\}^n$, $n \in \mathbb{N}$ that fulfils the following optimal condition:

$$|x^*\rangle = \underset{|x\rangle \in \{0,1\}^n}{\operatorname{argmin}} \langle x|Q|x\rangle$$
 (1)

where the linear operator $Q \in \mathbb{R}^{n \times n}$ is a symmetric matrix. This can be interpreted as an objective function:

$$f_Q(x) = \langle x|Q|x\rangle = \sum_{i=1}^n \sum_{j=i}^n Q_{ij}x_ix_j \qquad (2)$$

In general, QUBO is also NP hard due to the exponential scaling of the solution space in $\|\{0,1\}^n\|\in\mathcal{O}(2^n)$ with respect to the number of dimensions n. Many combinatorial optimisation problems have conversions into QUBO, not least the VRP and its variants. These conversions are useful to establish a uniform problem description for solvers to work with, however in the context of quantum solvers, they are further motivated by the equivalence between QUBO and the Hamiltonian of the Ising model for ferromagnetism in particle physics.

The Ising model describes a lattice structure Λ in which each lattice site houses a particle. The spin of each particle is represented by a discrete variable $\sigma_i \in \{-1,1\}$, $i \in \Lambda$. This spin value governs the local magnetic moment of the particle according to the shell model (appendix). Neighbouring lattice sites $\langle i j \rangle$. $i, j \in \Lambda$ influence each other, termed nearest neighbour interactions, whose interaction strength is represented by $J_{ij} \in \mathbb{R}$. Furthermore, one may consider the influence of an external field h_i at site $i \in \Lambda$, such that the spin wants to align with this field.

Thus the Hamiltonian reads:

$$H = -\sum_{\langle i j \rangle} J_{ij} \sigma_i \sigma_j - \mu \sum_i h_i \sigma_i \tag{3}$$

where μ is the magnetic moment.

Replacing σ with the Pauli operators yields the quantum mechanical description:

$$H = -\sum_{\langle i j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \mu \sum_i h_i^z \sigma_i^z - \mu \sum_i h_i^x \sigma_i^x$$
 (4)

where the second term with σ^z describes the external longitudinal field, and the final term with σ^x describes the transverse field per lattice site.

Notably, the Ising model is typically simplified to exclude the transverse field, resulting in a classical Hamiltonian where the constituent terms commute ie. a diagonal operator in the Z basis. This

means the ground state is described by a basis vector $|\phi\rangle$ with $\phi \in \{0,1\}^n$, allowing for simple measurement to obtain a bit string solution.

Through the reversible transformation $\sigma \mapsto 2x-1$, where $x \in \{0,1\}$ s.t. $-1 \mapsto 0$ and $1 \mapsto 1$, one obtains the equivalent QUBO formulation for free, and hence optimising for the ground state of the Ising Hamiltonian is equivalent to optimising the QUBO objective function.

IV. Encoding Approaches

A simple mapping from the VRP to QUBO uses what is known as the complete encoding, where each classical binary variable is represented by a single qubit.

V. Discussion

VI. Conclusion

References

VII. Appendix

$$C(\theta) = \langle H \rangle = \langle \psi(\theta) | H | \psi(\theta) \rangle \tag{5}$$