Combinatorial Optimisation with Adiabatic Quantum Computing

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08 September 2023

Combinatorial optimisation is the act of finding the **ideal combination** of a discrete set of objects subject to a set of **constraints**; its applications span biology, engineering, computer science, and applied mathematics. In this work, we solve the combinatorial optimisation problem **Maximal Independence Set** for a small 5-vertex graph with **Adiabatic Quantum Computing** simulated in Python, and suggest that a $t_{\max}$ of **18** is optimal, giving a success probability of **0.99** in line with the industry standard (King, J. et al., 2015).

1 Optimisation

Combinatorial optimisation (CO) is the act of finding the **ideal combination** of a **discrete** set of objects subject to a set of **constraints**. CO problems are found everywhere, from protein structure prediction in biology, to delivery scheduling in logistics[1].

In theory, all CO problems can be solved if every possible solution is calculated and compared, but, unfortunately, their sets of possible solutions often grow exponentially with problem size, making this intractable. Instead, we look to more efficient **heuristic** algorithms that yield approximate solutions. CO is a large area of research, with many classical algorithms able perform it relatively efficiently[2]. For a quantum approach to be worthwhile, it is not sufficient to demonstrate it performs CO: a clear advantage over classical approaches must be shown in order to justify the hardware investment required.

In this work, we solve the CO problem **Maximal Independent Set** (MIS) with simulated Adiabatic Quantum Computing, demonstrating that it could be solved on a real Adiabatic Quantum Computer. For a graph of n vertices, some connected by edges, the MIS is obtained by colouring **as many vertices as possible** whilst requiring that **no two coloured vertices** are **connected** by an edge. MIS has broad applications, from financial analysis, to digital error correction[3]. **Fig. 1** shows the MIS of the graph we investigated, defined by upper-triangular adjacency matrix M, where elements M_{ij} are 1 if vertices i and j share an edge, and else 0. This graph has $2^5 = 32$ possible colourings.

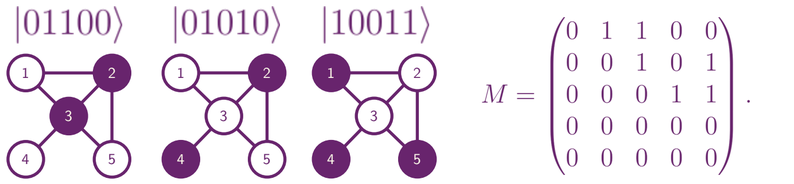

Fig. 1: The graph we investigated. From left to right: a coloured set which isn't independent, is independent but not maximal, the maximal independent set, the adjacency matrix that defines the graph. The graphs are annotated with the state vectors describing their colouring.

2 Adiabatic Quantum Computing (AQC)

AQC is a form of quantum computing based on the Quantum Adiabatic Theorem: *an isolated physical system **prepared in the ground-state** of a time-dependent Hamiltonian **stays in the ground-state** as time evolves and the Hamiltonian changes, provided the change is sufficiently small and there is always a sufficient energy gap between the ground and first-excited states*[4]. In AQC, the time-dependent Hamiltonian is the sum of two terms,

$$H(t) = A(t)H_{\text{initial}} + B(t)H_{\text{problem}}. \tag{1}$$

The initial Hamiltonian, H_{initial}, has a **known ground-state** in which the system is prepared. The final, problem Hamiltonian, H_{problem}, is chosen such that its **ground-state describes** the **optimal solution**. $H(t)$ is a 2^n x 2^n matrix, so its ground-state is difficult to calculate for a large number of vertices n. Instead, we can use AQC to find the ground state of H_{problem}, and thus perform CO. In this work, we chose to set

$$A(t) = 1 - t/t_{\max} \quad \text{and} \quad B(t) = t/t_{\max}, \tag{2}$$

where $t_{\max}$ is the total time the system takes to solve the problem. For an ideal Adiabatic Quantum Computer, $t_{\max} \to \infty$, but, as we show, **the process works heuristically** for **finite time periods**, giving the optimal solution 99% of the time for a $t_{\max}$ of 18.

3 The Ising Model

To solve a CO problem with AQC, we must define a Hamiltonian H_{problem} whose **ground-state describes the optimal solution**. For this, we borrow the **Ising model** from statistical mechanics. The Ising Hamiltonian is given by

$$H_{\text{Ising}} = \sum_{k=1}^{n}\sum_{j=k+1}^{n} J_{kj}\sigma_k^z\sigma_j^z + \sum_{j=1}^{n} h_j\sigma_j^z, \tag{3}$$

where

$$\sigma_j^z = \left(\bigotimes_{k=1}^{j-1} I_2\right) \otimes \sigma^z \otimes \left(\bigotimes_{k=j+1}^{n} I_2\right), \tag{4}$$

I_2 is the 2 x 2 identity matrix, n the total number of vertices, σ^z the z-th Pauli matrix, and h_j and J_{kj} are **chosen specifically for each problem**[5]. $\bigotimes$ denotes sequential tensor products. We encoded our problem into the Ising Hamiltonian, setting $J = M$, and

$$h_k = -\sum_{j=1}^{n}(M_{kj} + M_{jk}) + \kappa, \tag{5}$$

where $\kappa = 1/2$ was added to **reward** (give lower energy for) a **higher number of coloured vertices**, and J and h_k were chosen to **reward independence**[6].

4 Simulation

We simulated the process with matrix techniques in Python, using NumPy and SciPy for linear algebra operations, setting

$$H_{\text{initial}} = -\sum_j \sigma_j^x \tag{6}$$

and $H_{\text{problem}} = H_{\text{Ising}}$ as defined above. We initialised the wavefunction in the ground-state of H_{initial}, $|\psi(t=0)\rangle$, and **simulated time evolution** using the exponential **time-evolution operator** derived from Schrodinger's equation, finding the wavefunction after k steps to be

$$\left|\psi\left(t = \frac{kt_{\max}}{q}\right)\right\rangle \approx \mathcal{T}\prod_{j=1}^{k}\exp\left[-i\frac{t_{\max}}{q}H\left(\frac{jt_{\max}}{q}\right)\right]|\psi(t=0)\rangle \tag{7}$$

where $\mathcal{T}$ indicates the products are time-ordered, and q gives the total number of steps the simulation takes. The formula is exact in the limit q goes to infinity, but for our purposes we found $q = 1000$ to yield good results.

Since $H(t)$ lives and acts in the space of 2^n-component column vectors, $|\psi\rangle$ can always be expressed as a **linear combination** of the column vectors $|j\rangle$, the standard basis vectors with 1 at index j, and 0 elsewhere. From **Fig. 1**, we know the **ground-state of our H_{Ising}** to be $|10011\rangle = |19\rangle$, representing the MIS. From the quantum measurement theory, the probability of measuring a system with wavefunction $|\psi(t)\rangle$ in state $|j\rangle$ at time t is given by

$$P\left(|j\rangle; |\psi(t)\rangle\right) = |\langle j|\psi(t)\rangle|^2 \implies P_{\text{s}}(t) = |\langle 19|\psi(t)\rangle|^2, \tag{8}$$

where $P_{\text{s}}(t)$ gives the probability of success.

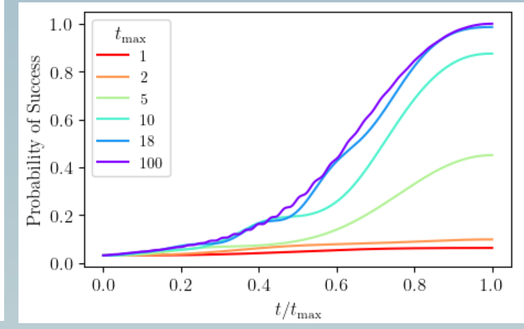

Fig. 2: Instantaneous probability of success in finding the MIS of the graph we investigated, plotted for six values of $t_{\max}$.

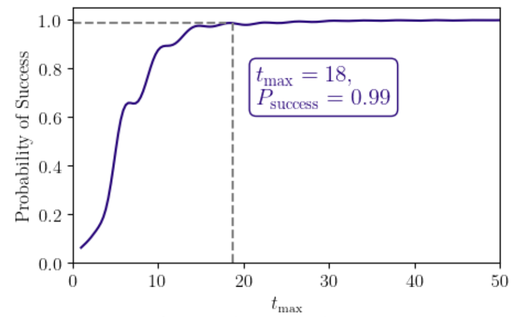

Fig. 3: Probability of success for values of $t_{\max}$ between 1 and 50. The optimal value of $t_{\max}$ we determined, 18, is indicated, along with its associated success probability of 0.99.

SCAN to see how the probability of measuring the system in each $|j\rangle$ changes during simulation for $t_{\max} = 18$.

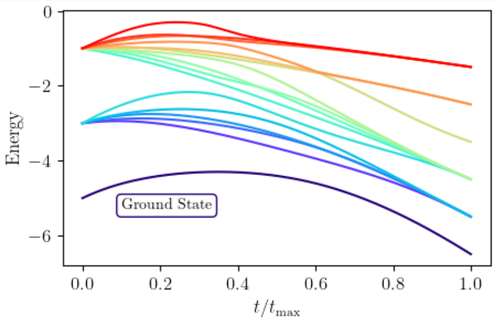

Fig. 4: Instantaneous energy eigenspectrum of the system we investigated. States higher than the initial third excited state omitted for clarity. The energy gap between the ground and first-excited states is sufficient for the process to be adiabatic throughout.

In **Fig. 2**, the instantaneous probability of success, $P_{\text{s}}(t)$, is plotted for six values of $t_{\max}$. In **Fig. 3**, the final probability of success was plotted for values of $t_{\max}$ between 1 and 50. **At values of $t_{\max}$ close to 1**, the success probabilities weren't far removed from **random guessing**. The algorithm got more successful as $t_{\max}$ increased up to approximately 18, after which it stayed approximately constant between 0.99 and 1. We can therefore say that the process was **approximately adiabatic** for $t_{\max}$ in this range, meaning the evolution was sufficiently slow, and the energy gap between the ground and first-excited states was sufficiently large, as shown in **Fig. 4**, for the Quantum Adiabatic Theorem to apply.

Success probabilities of 0.99 or greater are generally perceived as acceptable in industry, so we determine, from **Fig. 3**, $t_{\max} = 18$ to be the optimal choice [7], and state that AQC can be used to find the MIS for our graph **heuristically**.

The graph we investigated was small and **could be easily solved classically**. To prove AQC is viable as a method for CO, some kind of *'quantum advantage'* must be demonstrated over classical approaches, either producing the same results in a shorter time-period, or producing better results in the same time-period. We **did not demonstrate** any **quantum advantage** in this work.

References

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