Grover's Quantum Algorithm and the Maximum Clique Problem

Matheus Giovanni Dias[a,b], Leandro Miranda Zatesko[a,b]

[a] *Academic Department of Informatics, Federal University of Technology — Paraná, Curitiba, Brazil*
[b] *Emails: matheusdias@alunos.utfpr.edu.br, zatesko@utfpr.edu.br*

Abstract

The Maximum Clique Problem consists of finding in a simple graph the largest subset of vertices wherein each pair of vertices is connected by an edge. It is an NP-Hard problem with many practical applications. In this paper we show how to implement an oracle for Grover's Quantum Search, yielding a quantum algorithm for finding the maximum clique in an n-vertex simple graph. The yielded algorithm has overall time complexity $\mathcal{O}(\sqrt{2^n}(n \log n)^2)$ and space complexity $\mathcal{O}(n^2)$.

Keywords: Vertex subsets with special properties, Quantum algorithms and complexity in the theory of computing, Graph algorithms
2020 MSC: 05C69, 68Q12, 05C85

1. Introduction

In graph theory, a *clique* in a simple graph is a subset of vertices wherein every pair of distinct vertices are adjacent (connected by an edge). Throughout this text, a graph is always a simple graph. A *maximal* clique is a clique that is not contained in a larger clique in the same graph. A *maximum* clique is a largest maximal clique of a graph. Determining the cardinality of the maximum clique in a graph is a well-known NP-Hard problem [1]. The best-known classical algorithm for this problem has time complexity $\mathcal{O}(3^{\frac{n}{3}})$. The Maximum Clique Problem is also hard to approximate [2], i.e. for any $\varepsilon > 0$, there cannot be a polynomial-time approximation algorithm for the problem within an $\mathcal{O}(n^{1-\varepsilon})$ approximation factor, unless $\mathsf{P} = \mathsf{NP}$.

Grover's Quantum Search is a quantum[1] search algorithm that provides a polinomial speedup over the best-known classical solutions for several important problems. This algorithm uses the quantum superposition and interference phenomena to search in a set of possible solutions for a value x that *satisfies* a black-box Boolean function $f : \{0,1\}^n \to \{0,1\}$, referred to as the *oracle* for the problem, that is, $f(x) = 1$ when x is a solution for the

[1] We refer the reader to: Nielsen and Chuang [3] for preliminaries on Quantum Computing and Quantum Mechanics; Diestel [4] for preliminaries on Graph Theory.

problem, and $f(x) = 0$ otherwise. After $\mathcal{O}(\sqrt{2^n})$ evaluations of the function, the probability that a solution is found is $1 - \mathcal{O}(1/n)$.

Bojié [5] proposed an algorithm based on Grover's Quantum Search for finding a maximum clique in a simple graph G. He uses an iterative approach for searching a clique in a list of subgraphs with at least k vertices, starting at $k = 1$. For each iteration k, the clique is found by running a Grover's Search. After each iteration, the value of k is incremented until no clique is found. The author mentions the use of a binary search instead an iterative approach to speedup the algorithm by a $\log n$ factor. However, the author does not provide the implementation of the oracle for the Grover's Search. They do not even consider the complexity of the construction of such oracle; only its description is provided:

$$f(x) = \begin{cases} 1, & \text{if } x \text{ encodes a maximal clique with at least } k \text{ elements;} \\ 0, & \text{otherwise.} \end{cases}$$

Wie [6] proposed an algorithm based on Grover's Quantum Search for finding all maximal (not necessarily maximum) cliques in a graph G. The algorithm returns a superposition of all quantum states that describe a maximal clique in G. The author includes the description of the oracle, alongside with the instructions for creating the quantum circuit:

$$f(x) = \begin{cases} 1, & \text{if } x \text{ encodes a maximal clique;} \\ 0, & \text{otherwise.} \end{cases}$$

Since a maximum clique is a maximal clique, we can use Wie's oracle in Bojié's algorithm if the input state for Wie's oracle consists of a superposition of all states that encode a subgraph of G with at least k vertices.

In this paper we show how to prepare this input state for Wie's oracle, leading to an $\mathcal{O}(\sqrt{2^n}(n \log n)^2)$-time quantum algorithm for solving, with high probability, the Maximum Clique Problem. Remark that this is better than the $\mathcal{O}(3^{\frac{n}{3}})$ classical time, since

$$\lim_{n \to +\infty} \frac{\sqrt{2^n}(n \log n)^2}{3^{\frac{n}{3}}} = 0\,. \tag{1}$$

It is also observed that the performance gain, compared to the classical solution, is lower than the maximum square gain that Grover's algorithm can provide, since $\left(\sqrt{2^n}(n \log n)^2\right)^2 > 3^{\frac{n}{3}}$ for $n > 1$. Furthermore, our algorithm not only returns the cardinality of a maximum clique, but also a superposition of all quantum states which encode a maximum clique in the graph.

2. The algorithm

We present an algorithm to prepare a quantum state that is a superposition of all states that encode a clique candidate in G with at least k vertices, being k a fixed positive integer.

A clique candidate C in a graph $G(V, E)$ is encoded as a binary string $|x\rangle = |x_1 x_2 ... x_n\rangle$ with $n = |V|$ qubits, wherein each qubit represents a vertex v_i of G and has the value:

$$|x_i\rangle = \begin{cases} |1\rangle\,, & \text{if } v_i \in C; \\ |0\rangle\,, & \text{otherwise.} \end{cases} \tag{2}$$

Note that a clique candidate with k vertices has exactly k qubits in the state $|1\rangle$. So, to find out the number of vertices in a clique candidate, we need to count the number of qubits in state $|1\rangle$. If this is done on a unary basis, the problem comes down to an ordering of the qubits in the binary string. In the unary basis we can also see if a clique candidate has at least k vertices by verifying if the k^{th} least significant qubit is in the state $|1\rangle$.

To count, on a unary basis, the number of qubits in the state $|x\rangle$ in a binary quantum string, we have developed a quantum algorithm based on the classical *insertion sort* algorithm. Substrings are iteratively ordered and expanded by inserting the remaining elements in the correct position. Each element inserted is either placed at the end of the string (most significant part), if it has value $|0\rangle$, or moved to the beginning (least significant part) if it has value $|1\rangle$. This quantum circuit can be constructed with CNOT and CSWAP gates, as described in Algorithm 1 and depicted in Figure 1.

Algorithm 1 Unary Qubit Counter

Input: $|x\rangle\,|a\rangle$; wherein $|a\rangle = |00\ldots0\rangle$

Output: $|x\rangle\,|u\rangle$; wherein $|u\rangle$ is a unary counting of the qubits of $|x\rangle$ in the state $|1\rangle$

for $i \in [1, 2, \ldots, n]$ **do**
    apply a CNOT gate controlled by $|x_i\rangle$, targeting $|a_i\rangle$;
end for
for $i \in [2, 3, \ldots, n]$ **do**
    for $j \in [i, i-1, \ldots, 2]$ **do**
        apply a CSWAP gate controlled by $|x_i\rangle$, targeting $|a_j\rangle$ and $|a_{j-1}\rangle$;
    end for
end for

The procedure for generating a superposition of all states with at least k vertices is based on another Grover's Quantum Search. This procedure aims to boost up the amplitude of the states in the superposition $|x\rangle$ that represent a clique candidate with at least k vertices. The oracle for this Grover's Search is depicted in Figure 2. The circuit is divided in 4 stages: *Copy to ancilla*, *Count in unary*, *Apply function* and *Clear ancilla*. The two first stages form the unary qubit counter (Figure 1). In the third stage we apply the function to the quantum state in a phase shift codification, as required by Grover's Algorithm, where the phase of the quantum input state $|x\rangle$ is inverted if $f(x) = 1$. This is done by applying a CNOT gate

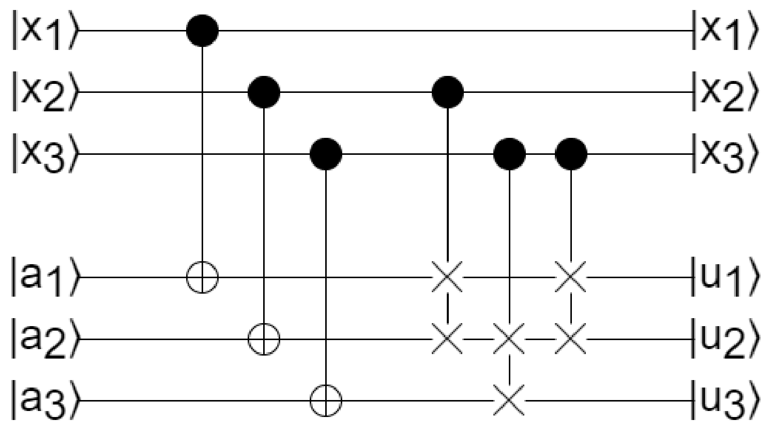

Figure 1: Unary qubit counter for $n = 3$

targeting a qubit in $|-\rangle$ state and controlled by a qubit $|c\rangle$ such that:

$$|c\rangle = \begin{cases} |1\rangle, & \text{if } f(x) = 1; \\ |0\rangle, & \text{otherwise.} \end{cases} \tag{3}$$

In this case, $|c\rangle$ is the k^{th} least significant qubit in the unary counting. In the last stage, the ancilla register is cleared by using a reversed circuit of the two first stages. Mathematically, the quantum circuit for this oracle O can be expressed as:

$$O|x\rangle = (-1)^{f(x)}|x\rangle . \tag{4}$$

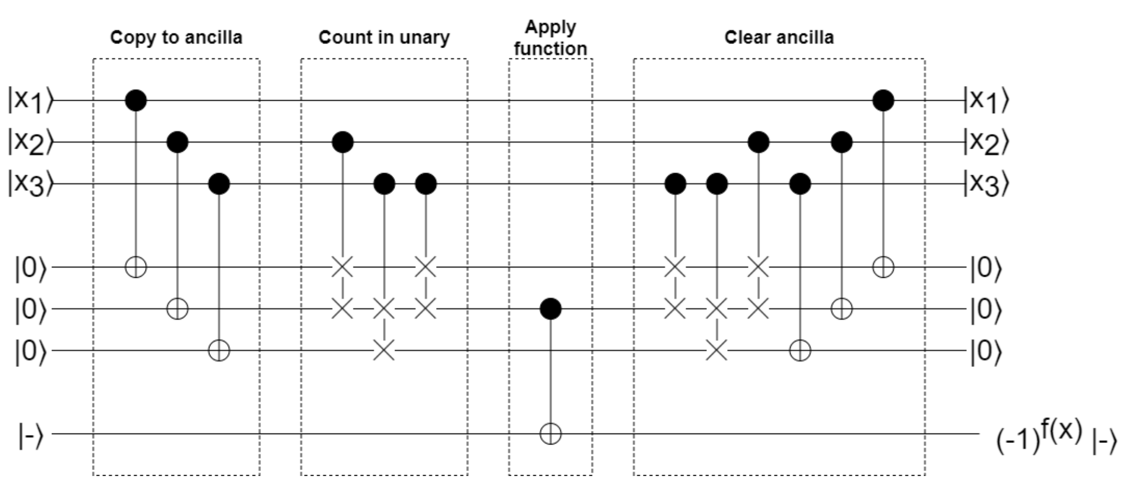

Figure 2: Quantum circuit for the oracle of the Grover's Search to generate the superposition of all clique candidates, with $n = 3$ and $k = 2$

The Grover's Search will leave the states that do not satisfy the oracle with a low amplitude. We can remove these states from the superposition by the use of quantum collapse and quantum entanglement phenomena. By adding another unary qubit counter at the end of the circuit and measuring the k^{th} least significant qubit of the counting, henceforth $|r\rangle$, the system will collapse, and the register $|x\rangle$ will be leaved in a superposition of all desired states if $|r\rangle = |1\rangle$, or an a superposition of all undesired states if $|r\rangle = |0\rangle$, according to the quantum entanglement phenomena. By Grover's effect, $|r\rangle$ will have a high probability of collapsing in $|1\rangle$, so we can repeat all the procedures until $|r\rangle$ collapses in $|1\rangle$ and $|x\rangle$ will be in the desired state of a superposition of all states with at least k qubits in $|1\rangle$. The full circuit for this algorithm is depicted in Figure 3.

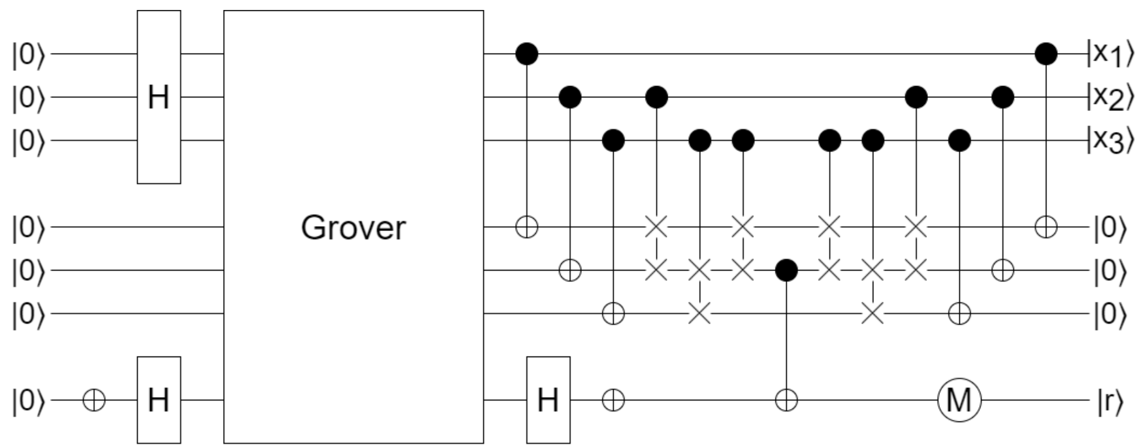

Figure 3: State generator for $n = 3$ and $k = 2$. The measurement is identified in the circuit by letter 'M'.

3. Brief analysis

Recall that our approach uses a binary search to make $\mathcal{O}(\log n)$ guesses for the value of k, building, for each guess, a circuit in $\mathcal{O}(n^2)$ time to prepare the input state for Wie's oracle through a Grover's Search, and then running another Grover's Search as in Wie's paper. This would yield an overall $\mathcal{O}(\sqrt{2^n} n^2 \log n)$ time complexity, but, to guarantee an overall $1 - \mathcal{O}(1/n)$ probability of error, each Grover's Search must be repeated some times.

Clearly, the probability p that our approach succeeds is bounded below by the probability that every Grover's Search individually and independently succeeds. Let p_i be the probability of success of the i^{th} Grover's Search, for $1 \leq i \leq 2\lceil \lg n \rceil$. To get $p \geq 1 - \mathcal{O}(1/n)$, as desired, it suffices to have each $p_i \geq (1 - \mathcal{O}(1/n))^{1/(2\lceil \lg n \rceil)}$, which we claim to be achieved by running each Grover's Search $\lfloor \lg n \rfloor$ times. The claim follows by observing that the probability that all these $\lfloor \lg n \rfloor$ iterations of Grover´s Search fail is $\mathcal{O}((1/n)^{\lg n})$, which is less than $1 - (1 - \mathcal{O}(1/n))^{1/(2\lceil \lg n \rceil)}$ for sufficiently large n. We have, then, our main result.

Theorem 1. *There is an $\mathcal{O}(\sqrt{2^n}(n \log n)^2)$-time and $\mathcal{O}(n^2)$-space quantum algorithm which, given an n-vertex graph G, outputs, with $1 - \mathcal{O}(1/n)$ probability of success, a state which is the superposition of all states which encode a maximum clique in G.* □

4. Final remarks

During the reviewing process, one of the reviewers pointed to us that a more efficient solution using Grover's algorithm for the Maximum Clique Problem could be achieved by an optimization algorithm such as the ones presented in [7] and [8]. For future work, we aim to investigate this reviewer's suggestion.

Acknowledgements

We thank the anonymous referee for the valuable suggestions given.

References

[1] R. M. Karp, Reducibility among combinatorial problems, Complexity of Computer Computations (1972) 85–103.

[2] J. Håstad, Clique is hard to approximate within $n^{1-\epsilon}$, Acta Math 182 (1999) 105–142. doi:10.1007/BF02392825.

[3] M. Nielsed, I. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, 2000.

[4] R. Diestel, Graph Theory, Springer-Verlag, New York, 1997.

[5] A. Bojié, Quantum algorithm for finding a maximum clique in an undirected graph, JIOS 36 (2012) 91–98.

[6] C. R. Wie, A quantum circuit to construct all maximal cliques using Grover search algorithm, arXiv: Quantum Physics (2017). URL: `https://arxiv.org/abs/1711.06146`.

[7] C. Dürr, P. Høyer, A quantum algorithm for finding the minimum, 1996. URL: `https://arxiv.org/abs/quant-ph/9607014`.

[8] L. A. B. Kowada, C. Lavor, R. Portugal, C. M. H. Figueiredo, A new quantum algorithm for solving the minimum searching problem, International Journal of Quantum Information 6 (2008) 427–436.