Quantum Search Algorithms on Hierarchical Networks

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Abstract—The "abstract search algorithm" is a well known quantum method to find a marked vertex in a graph. It has been applied with success to searching algorithms for the hypercube and the two-dimensional grid. In this work we provide an example for which that method fails to provide the best algorithm in terms of time complexity. We analyze search algorithms in degree-3 hierarchical networks using quantum walks driven by non-groverian coins. Our conclusions are based on numerical simulations, but the hierarchical structures of the graphs seems to allow analytical results.

I. INTRODUCTION

Searching algorithms play an important role in quantum computing. One of the best-known quantum algorithms is due to Grover [1], which allows one to find a marked item in an unsorted database quadratically faster compared with the best classical algorithm. It uses an important technique called amplitude amplification, which can be applied in many computational problems providing gain in time complexity.

A related problem is to find a marked location in a spatial, physical region. Benioff [2] asked how many steps are necessary for a quantum robot to find a marked vertex in a two-dimensional grid with N vertices. In his model, the robot can move from one vertex to an adjacent one spending one time unit. Benioff showed that a direct application of the Grover algorithm does not provide improvements in the time complexity compared to a classical robot, which is O(N). Using a different technique, called *abstract search algorithms*, Ambainis et. al. [3] showed that it is possible to find the marked vertex with $O\left(\sqrt{N}\log N\right)$ steps. Tulsi [4] was able to improve this algorithm obtaining the time complexity $O\left(\sqrt{N\log N}\right).$

The time needed to find a marked vertex depends on the spatial layout. The abstract search algorithm is a technique that can be applied to any regular graph. It is based on a modification of the standard discrete quantum walk. The coin is the Grover operator for all vertices except for the marked one which is -I. The choice of the initial condition is also essential. It must be the uniform superposition of all states of the computational basis of the coin-position space. This technique was applied with success on higher dimensional grids [3], honeycomb networks [5], regular lattices [6] and triangular networks [7].

In this work, we analyze a hierarchical network called Hanoi

network (HN3) [8], for which the abstract search algorithm does not provide the most efficient search algorithm. HN3 is a special case of small world networks, which are being used in many contexts including quantum computing [9], [10]. In order to obtain a quicker algorithm, we modify the coin operator and the initial condition used in the abstract search algorithm to take advantage of the small world structure. Our results are based on numerical simulations, but the hierarchical structure of HN3 indicates that analytical results can also be obtained.

The structure of the paper is as follows. Sec. II introduces the degree-3 Hanoi network. Sec. III describes the standard coined discrete quantum walk on HN3. Sec. IV reviews the basics of the abstract search algorithm. Sec. V describes the modifications we propose to enhance the time complexity of quantum search algorithms on HN3. Sec. VI describes the main results based on numerical simulations. Finally, we present our conclusion in Sec. VII.

II. HIERARCHICAL STRUCTURES

The Hanoi network has a cycle with $N = 2^n$ vertices as a backbone structure, that is, each vertex is adjacent to 2 neighboring vertices in this structure and extra, long-range edges are introduced with the goal of obtaining a small-world hierarchy. The labels of the vertices $0 < k \leq 2^n - 1$ can be factorized as

$$k = 2^{\kappa_1} (2k_2 + 1), \tag{1}$$

where k_1 denotes the level in the hierarchy and k_2 labels consecutive vertices within each hierarchy. In any level, one links the vertices with consecutive values of k_2 keeping the degree constraint. When $k_1 = 0$, the values of k are the odd integers. For HN3, we link 1 to 3, 5 to 7 and so on. The vertex with label 0, not being covered by Eq. (1), is linked to the vertex of label 2^{n-1} . Fig. 1 shows all edges for HN3 when the number of vertices is 16. Using this figure, one can easily built HN3 recursively, each time doubling the number of vertices. Our analysis will be performed for a generic value of n to allow us to determine the computational cost as function of N.

HN3 has a small-world structure because the diameter of the network only increases with $\sim \sqrt{N}$ [8], less fast than the number of vertices N. Yet, HN3 is a regular graph of fixed degree d = 3 at each vertex.

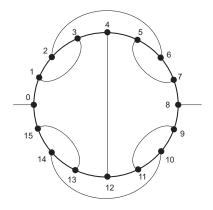


Fig. 1: HN3 with 16 vertices.

III. QUANTUM WALKS ON HIERARCHICAL STRUCTURES

A coined quantum walk in HN3 with $N = 2^n$ vertices has a Hilbert space $\mathcal{H}_C \otimes \mathcal{H}_P$, where \mathcal{H}_C is the 3-dimensional coin subspace and \mathcal{H}_P the N-dimensional position subspace. A basis for \mathcal{H}_C is the set $\{|a\rangle\}$ for $0 \le a \le 2$ and \mathcal{H}_P is spanned by the set $\{|k\rangle\}$ with, $0 \le k \le N - 1$. We use the decomposition $k = (k_1, k_2)$, given by Eq. (1), when convenient. A generic state of the discrete quantum walker in HN3 is

$$|\Psi(t)\rangle = \sum_{a=0}^{2} \sum_{k=0}^{N-1} \psi_{a,k}(t) |a\rangle |k\rangle.$$
 (2)

The evolution operator for the standard quantum walk [11] is

$$U = S \circ (C \otimes I), \tag{3}$$

where I is the identity in \mathcal{H}_P and S is the shift operator defined by

$$S |0\rangle |k_1, k_2\rangle = |0\rangle |k_1, k_2 + (-1)^{k_2}\rangle,$$

and

$$\begin{array}{lll} S \left| 1 \right\rangle \left| k \right\rangle & = & \left| 2 \right\rangle \left| k + 1 \right\rangle, \\ S \left| 2 \right\rangle \left| k \right\rangle & = & \left| 1 \right\rangle \left| k - 1 \right\rangle. \end{array}$$

The arithmetical operations on the second ket is performed modulo N. The shift operator obeys $S^2 = I$. C is a unitary coin operation in \mathcal{H}_C . In the standard walk, C is the Grover coin, denoted by G,

$$G = \frac{1}{3} \begin{bmatrix} -1 & 2 & 2\\ 2 & -1 & 2\\ 2 & 2 & -1 \end{bmatrix},$$
 (4)

which is the most diffusive coin [12].

For example, using Figure 1 we see that

$$S |0, 2\rangle = |0, 6\rangle$$

$$S |1, 4\rangle = |2, 5\rangle$$

$$S |2, 5\rangle = |1, 4\rangle$$

If the value of the coin is zero, the walker takes the edge that leaves the main circle. If the value of the coin is 1, the walker goes clockwise and inverts the value of the coin $(1 \rightarrow 2)$. If the value of the coin is 2, the walker goes counterclockwise and inverts the value of the coin $(2 \rightarrow 1)$.

The dynamics of the standard quantum walk is given by

$$|\Psi(t)\rangle = U^t |\Psi_0\rangle, \qquad (5)$$

where $|\Psi_0\rangle$ is the initial condition. After t steps of unitary evolution, we perform a position measurement which yields a probability distribution given by

$$p_{k} = \sum_{a=0}^{2} \left| \langle a, k | U^{t} | \Psi_{0} \rangle \right|^{2}.$$
 (6)

IV. ABSTRACT SEARCH ALGORITHMS

The abstract search algorithm [3] is based on a modified evolution operator $U' = S \cdot C'$, obtained from the standard quantum walk operator U by replacing the coin operation C with a new unitary operation C' which is not restricted to \mathcal{H}_C and acts differently on the searched vertex. The modified coin operator is

$$C' = -I \otimes |k_0\rangle \langle k_0| + C \otimes (I - |k_0\rangle \langle k_0|), \tag{7}$$

where k_0 is the marked vertex in a regular graph and C is the Grover coin G, the dimension of which depends on the degree of the graph. Ambainis et. al. [3] have shown that the time complexity of the spatial search algorithm can be obtained from the spectral decomposition of the evolution operator U of the unmodified quantum walk, which is usually simpler than that of U'.

The initial condition $|\psi_0\rangle$ is the uniform superposition of all states of the computational basis of the whole Hilbert space. This can be written as the tensor product of the uniform superposition of the computational basis of the coin space with the uniform superposition of the position space. Usually, this initial condition can be obtained in time $O(\sqrt{N})$, where N is the number of vertices.

The evolution operator is applied recursively starting with the initial condition $|\psi_0\rangle$. If t_f is the running time of the algorithm, the state of the system just before measurement is $U^{t_f} |\psi_0\rangle$. If one analyzes the probability of obtaining the marked vertex k_0 as function of time since the beginning of the algorithm, one gets an oscillatory function with the first maximum at t_f .

V. MODIFIED METHOD

The coin in a quantum walk is used to determine the direction of the movement. The Grover coin is an isotropic operator regarding all outgoing edges from a vertex. It is useful in networks that have no special directions, such as two-dimensional grids and hypercubes. The Hanoi network, on the other hand, has a special direction that creates the small world structure. Any edge that takes the walker outside the circular backbone provides an interesting opportunity in terms of searching. The strategy is to have a parameter that can control the probability flux among the edges, reinforcing or decreasing the flux outwards or inwards the circular backbone.

Instead of using the Grover coin of the *abstract search algorithms*, we use

$$C = \frac{2\epsilon}{d} |0\rangle \langle 0| + 2\sqrt{\frac{\epsilon(d-\epsilon)}{d^2(d-1)}} \sum_{j=1}^{d-1} (|j\rangle \langle 0| + |0\rangle \langle j|) + \frac{2(d-\epsilon)}{d^(d-1)} \sum_{j,j'=1}^{d-1} (|j\rangle \langle j'| + |0\rangle \langle j|) - I,$$
(8)

where d = 3 is the degree at each vertex. When $\epsilon = 1$, the Grover coin is recovered. When $0 < \epsilon < 1$, the probability flux along small-world edges which escapes from the circular backbone is weakened. When $1 < \epsilon < 3$, the probability flux off the backbone is reinforced, allowing the walker to use the small world structure with higher efficiency. Hence, this new coin controls the bias to escape off the circular backbone of HN3 through the parameter ϵ .

The *abstract search algorithms* use a uniform distribution as initial condition. We change this recipe. The initial condition is

$$\left|\psi(0)\right\rangle = \sqrt{\frac{\epsilon}{d}}\left|0\right\rangle\left|s\right\rangle + \sqrt{\frac{d-\epsilon}{d(d-1)}}\sum_{j=1}^{d-1}\left|j\right\rangle\left|s\right\rangle,\qquad(9)$$

where $|s\rangle$ is the uniform superposition on the position space. When $\epsilon = 1$ the initial condition is the uniform superposition of coin-position space.

The analysis of the evolution of the quantum search algorithm using the new coin and initial condition is far more complex than the standard one. Our conclusions here are based in numerical simulations. Since the standard abstract search algorithm with Grover coin is obtained with $\epsilon = 1$, our simulations allow us to compare the cost of the new search algorithm with the standard one and to determine the value of ϵ that optimizes the total cost of the algorithm.

VI. RESULTS

Fig. 2 shows the oscillatory behavior of the probability of finding the walker at the marked vertex k_0 . Initially, the probability is close to zero, because the initial condition is a state that is close to the uniform superposition of all vertices. The running time of the algorithm is the value of t for which the probability reaches its first maximum. Note that for $\epsilon = 1$, which is the *abstract search algorithm*, the maximum value of the probability is smaller than that of $\epsilon = 2$. The maximum value for $\epsilon = 2$ occurs at a time latter than that of $\epsilon = 1$. This is not a problem, as we show when we analyze the total cost of the algorithm. In either case, the maximum value of the probability is not close to 1, as one would expect in order to have high probability to find the marked vertex. This means that the algorithm must be rerun many times to amplify the success probability.

Fig. 3 shows the success probability, defined as the first peak in Fig. 2, of a single run of the search algorithm as a function of the network size N for different values of ϵ . The horizontal axis is in logscale for better visualization. From the line inclination, we conclude that the success probability decays

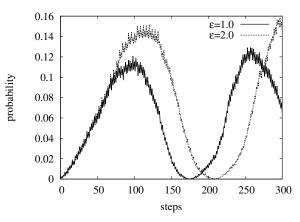


Fig. 2: Probability of finding walker at vertex k_0 as a function of time for two values of ϵ .

approximately as $O(1/\log N)$. It means that the algorithm must be rerun around $O(\log N)$ times in order to ensure a success probability close to 1.

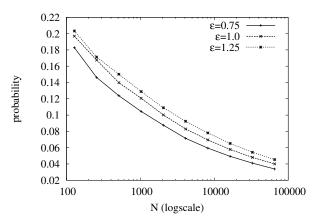


Fig. 3: Success probability of the search algorithm as a function of N for three values of $\epsilon.$

Fig. 4 shows the success probability as function of parameter ϵ for three values of N. The success probability is an increasing function in terms of ϵ . The range $\epsilon < 1$ is the worst one. This can be explained in the following way. For small values of ϵ , the walker is constrained to live in the HN3 backbone cycle. It is known that quantum and classical search algorithms in cycles have the same time complexity. On the other hand, in the range $\epsilon > 1$, the success probability is greater than the one obtained in the *abstract search algorithm*. Recall that when $\epsilon > 1$, the probability flux along small-world edges is reinforced. This is a strong indication that small world structures improve quantum search algorithms.

The perspective provided by Fig. 4 is incomplete for HN3, though. While the highest values of ϵ appear to be favorable, the analysis of the total cost of the algorithm points out to another value. Fig. 5 shows the computational cost of the search algorithm in terms of ϵ for three values of N. The minimum cost occurs for $\epsilon \approx 1.7$, which is well above the value for the Grover coin, $\epsilon = 1$. This clearly shows that the

abstract search algorithm does not provide the best algorithm for searching a marked vertex in the hierarchical structures. In turn, minimizing cost occurs also well below the value of ϵ that maximized probability. This discrepancy likely originates with the "confinement" effect already observed for a classical walker on HN3 [8]: To utilize ever-longer small-world edges off the backbone, a walker has to be able to mover ever further along the backbone between those edges. At exactly $\epsilon = 3$, the probability for moving along the backbone vanishes, and a walker remains confined to its present small-world edge and the cost in Fig. 5 diverges.

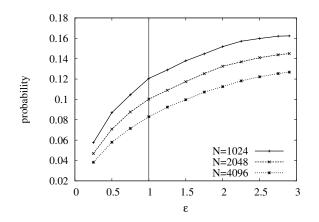


Fig. 4: Success probability as function of parameter ϵ for three values of N.

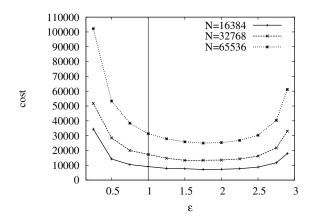


Fig. 5: Computational cost of the search algorithm in terms of ϵ for three values of N.

Naive analogy with the exact renormalization group (RG) analysis for the classical walker [8] would suggest that the cost of a quantum walk would be minimized in a boundary layer for $\epsilon \rightarrow 3$ with a width that decreases as some power of the system size N. Our simulations in Fig. 5 exhibit a very broad cost-minimum near $\epsilon \approx 1.7$, especially for small values of N. For the system size attained in our simulations, it is difficult to decide whether the minimum point will converge to a finite value of $\epsilon < 3$ or approach $\epsilon \rightarrow 3$ for large N. We are currently analyzing search algorithms on another Hanoi network, HN4 [8], which is 4-regular and does not suffer

confinement. While otherwise identical to HN3, in HN4 two small-world edges extend off the backbone symmetrically in *both* directions from each vertex.

Fig. 6 shows the computational cost of the search algorithm as a function of the network size N for different values of ϵ . Those plots complement the plot of Fig. 5. From the line inclination, we conclude that the cost is $O(N^c \log N)$, where c is a constant close to 0.8. It is clear from the plots that the curve corresponding to the lowest time complexity has $\epsilon > 1$, outperforming the Grover coin.

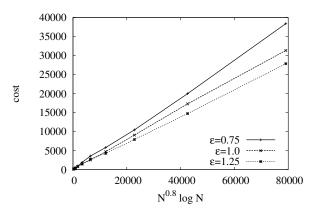


Fig. 6: Computational cost of the search algorithm in terms of $N^{0.8} \log N$ for three values of ϵ .

VII. CONCLUSION

The *abstract search algorithm* is a powerful technique for the development and analysis of quantum search algorithms on regular graphs. The quantum speed-up achieved by the abstract search algorithm strongly depends on the properties of the graph under consideration. In this work, we study the quantum search on the Hanoi network (HN3). This particular graph presents a sufficiently intricate structure to exhibit nottrivial properties for statistical models, yet sufficiently simple to reveal analytical insights.

We proposed a modification on the abstract search algorithm for HN3 and numerically analyzed its performance. Our modification consisted on changing the coin operator in order to have a parameter ϵ that controls the probability flux among the edges, enhanced either along or off the circular backbone. Our modified method also uses a parameterized initial condition instead of the uniform distribution.

Our numerical results clearly show that the performance of the search algorithm is better when we choose the parameter $\epsilon > 1$ to reinforce the probability flux along small-world edges instead of the circular backbone (which would correspond to $\epsilon < 1$). The success probability of a single run of the search algorithm is considerably higher whenever we choose $\epsilon > 1$. The total cost of the algorithm appears to reach a minimum for $\epsilon \approx 1.7$. The cost appears to scale with $\sim N^{0.8}$ with the system size. A more elaborate analysis used for the classical walker in Ref. [8] and for quantum transport through HN3 in Ref. [13] is required to provide exact results. We conclude that the abstract search algorithm, which uses the Grover coin to drive the quantum walk on a regular graph, does not provide the most efficient search algorithm for the Hanoi network HN3.

Our works on progress are now focused on the analysis of search algorithms for the Hanoi network HN4.

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