Quantum search with prior knowledge

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Abstract

The aim of this work is to develop a framework for realising quantum network algorithms with the use of prior knowledge about the structure of the network. We seek to obtain computational methods that allows us to locally determine network properties in a quantum superposition and drive the walk behaviour accordingly. In particular, we consider a network that consists of different types of edges, such that the transitions between nodes result in extra edge-dependent phase shift. We combine amplitude amplification and phase estimation to develop an algorithm for exploring such networks. In the layered neural network inspired case we obtain linear increase of the search complexity with exponential growth of the nodes number. We show that in consequence one is able to perform quantum search algorithms with exponential speed-up compared to quantum search that neglects the extra phase shifts.

Introduction

Quantum algorithms developed by Grover [1] and Shor [2] provide the highest motivation for exploring the computational possibilities offered by quantum mechanics. The crucial ingredients of the above algorithms, amplitude amplification in the case of quantum search and phase estimation in the case of quantum factorization, are important elements of most of the existing quantum algorithms [3,4,5].

In this work we focus on quantum search problems, in particular considering computation on trees as a problem instance. We aim at developing methods for harnessing additional knowledge during the search using heuristic methods. In particular, for broadening the heuristics potential, we try to obtain methods that allows one to model non-binary evaluation function enabling multi-threshold approach and ones that do not involve coin operator for evaluation input.

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For the given purpose we choose quantum walk model \([6, 7, 8]\) as one of the most promising, partially due to being universal for quantum computation \([9, 10]\) and relatively intuitive. Quantum search with quantum walk is a well studied field \([11]\). Apart from the basic case a number of structures has been considered for spatial search \([12, 13, 14, 15, 16]\). Additionally, techniques that allows to perform fixed point search \([17]\), with almost arbitrary operations \([18, 19]\), fault ignorant \([20]\) or a search without an oracle \([21]\) exists. Quantum search is also considered in context of quantum foundations \([22, 23]\).

In this work we start with consideration of quantum search on a tree \([24, 25]\), which is motivated by the fact that any connected network can be considered using spanning tree and tree graphs occur naturally in modelling decision problems.

The model we consider greatly depends on possibility to enable and disable connections due to its evaluation. Such mechanism is used in many contexts. One seeks a method to reduce the set of states e.g. by selecting a subspace, harnessing symmetries, and in consequence obtaining some kind of regularity in the structure \([26]\). Also, studying open systems is often done by simulating percolation, methods for dynamical control of underlying graph structure are of interest \([27]\). The methods presented in our work allow one to arbitrarily change connections by changing phase shifts in the network or its interpretation. We consider disabling one edge in a pair as restriction of direction according to one of the dimensions. One of the models where such restriction is present is so called self-avoiding walk which is an active field of research. In particular tunable self-avoidance is recently analysed \([28]\), which may be obtained for a walk with many different phase shifts with dynamically changing interpretation.

As brute force search complexity is bounded from below, the considered approach may work only when additional knowledge is accessible. In general it would be advantageous if quantum heuristics could be applicable for any NP hard problem \([29]\). Harnessing additional knowledge during the walk has been studied in context of discrete cellular automata, where e.g. feed-forward coin dependence is modelled \([30]\). Using some concepts of binary heuristics with tunable threshold in quantum tree search has been shown to be worth analysing in context of production systems and decision problems \([31]\). The possibilities of harnessing known heuristics methods for some class of classical problems, that provide better than quadratical speed-up and make quantum brute force methods useless in most of the problem instances has been studied for backtracking methods \([32]\) as well as a search with advice \([33]\). We highlight that the decisions made on the node during the walk are similar to the ones considered for mobile agents. The possibility to use agents affecting the measurement settings to improve quantum network exploration \([34]\) or search \([35]\) has been analysed and the authors lay out a path for adaptive controllers based on intelligent agents for quantum information tasks.

In this work we highlight the possibility to obtain non-binary evaluation function. Harnessing many different phase shifts allow many thresholds. Anal-
ysis of quantum inspired ways of multi-thresholding shows that it is beneficial for image processing [36].

It is also worth noting that also adiabatic quantum computation model has been modified in order to harness heuristic guesses [37]. Joining quantum and classical techniques into one procedure can also be beneficial even when the quadratical speed-up is lost by avoiding non-perfect randomness [38]. The idea can be applied also for purely quantum decision problems e.g. for oblivious set-member decision problem [39]. More advanced tasks one obtains a decision tree often may be characterized with use of a decision tree, which would fit into presented approach.

We combine amplitude amplification with phase estimation to develop a framework for exploring quantum networks. We introduce a model of quantum network which allows us to utilize information about the connections. We apply the introduced framework to develop a quantum walk search procedure exploiting the structural information in the network. We show that this search procedure allows one to obtain exponential speed-up over the quantum search procedure which does not utilize the information available in the network.

This work is organized as follows. In section the network and the walk model is introduced. In section we provide the algorithm and discuss the complexity. Section provides concluding remarks.

Network model

The results presented in this paper are based on the quantum walk model on a network that consists of various types of edges. We aim at encoding information about network structure into these types and extracting this knowledge during the computation.

Phase altering network

Let us consider a network of $n$ nodes with corresponding label set $V$ and edge set $E$. We assume that the degree of each node is equal to $d$ and describe the edge labelling by a function $D(x, y) = c \in \{1, \ldots, d\}$ for $(x, y) \in E$ such that $D(x, y) \neq D(x, y')$. For describing the dynamics of the system we use a quantum walk model [40] [11] [41]. The model described is consistent with the most general form used for implementing walks on various structures [13] [42] [14] [43] The corresponding quantum system is a Hilbert space $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_C$, $\mathcal{H}_p = \mathbb{C}^n$, $\mathcal{H}_C = \mathbb{C}^d$. Each basis state $|p, c\rangle = |p\rangle \otimes |c\rangle$ encodes position $p$ and direction $c$. The most commonly used shift operator takes the form

$$\sum_{(x,y) \in E} |y, D(y,x)\rangle \langle x, D(x,y)|.$$  

However, such model does not differentiate the edges. To achieve this effect we introduce a model in which the shift operator includes an edge-dependent
In order to implement operator $E$ behaviour, one can introduce auxiliary loops that mimic the desired counterpart of the shift operator by applying additional coin operator $C$. The two-shift operator $S^2$ exhibits unique phases $\varphi(x, y) + \varphi(y, x) < 2\pi$.

A network defined in such a way enables us to introduce a coin operator that utilizes the internal structure without using labels assigned to directions.

### Phase estimation within quantum walk

We use quantum phase estimation for computing phases resulting from shift operator application. In order to perform the phase estimation we include an additional memory register. We extend the Hilbert space with a qudit space $\mathcal{H}_M = \mathbb{C}^p$ so that the basis states are of the form $|x, c, m\rangle \in \mathbb{C}^n \otimes \mathbb{C}^d \otimes \mathbb{C}^p$. This enables us to include the auxiliary register for phase estimation and compute the phase label utilizing the Fourier basis on the memory register with $\mathcal{F} \in L(\mathbb{C}^p)$:

$$\mathcal{F}|k\rangle = \frac{1}{\sqrt{p}} \sum_{j=0}^{p-1} e^{i\varphi_k j} |j\rangle,$$

where $\varphi_k = \frac{2\pi k}{p}$ and $k = 0, \ldots, p-1$. We construct the phase estimation operator $E \in L(\mathcal{H}_P \otimes \mathcal{H}_C \otimes \mathcal{H}_M)$ using the controlled two shifts $S^2$ operator

$$E = (1_p \otimes 1_C \otimes \mathcal{F})\left(\sum_{j=0}^{p-1} (S^2)^j \otimes |j\rangle \langle j|\right).$$

In order to implement operator $E$ in a quantum walk scheme without altering the shift operator one can introduce auxiliary loops that mimic the desired behaviour.

auxiliary direction $c'$ for each direction $c$ such that $c'$ denotes an inactive counterpart of the $c$ direction ($S|x, c'\rangle = |x, c\rangle$). We control number of applications of the shift operator by applying additional coin operator that at step $l$ deactivates edges with state $|l\rangle$ at the memory register:

$$\sum_{j=0}^{p-1} (S^2)^j \otimes |j\rangle \langle j| = (1_p \otimes 1_{c\rightarrow c'} \otimes 1_M) \prod_{l=0}^{p-1} \left[(S^2 \otimes 1_M)D_l\right],$$

where we introduce active-inactive switch $1_{c\rightarrow c'} = 1_C - |c\rangle \langle c| - |c'\rangle \langle c'| + |c\rangle \langle c'|$ and controlled deactivation operator $D_l = \sum_{c=1}^{p-1} 1_p \otimes (1_{c\rightarrow c'} \otimes |l\rangle \langle l|) + 1_C \otimes \sum_{j \neq l} |j\rangle \langle j|$.

The two-shift operator $S^2$ has eigenvectors of the form $|x, y\rangle$ with eigenvalues $e^{2i\varphi(x, y)}$. Thus the phase estimation procedure $E$ results in

$$E: \frac{1}{\sqrt{p}} \sum_j |x, y, j\rangle \longrightarrow |x, y\rangle \otimes |\text{ph}(x, y)\rangle,$$
where $\varphi(x, y) = \frac{2\pi \text{ph}(x, y)}{p}$. As the result the label $\text{ph}(x, y)$ of the phase $\varphi(x, y)$ is encoded into the memory register.

**Proof of concept search algorithm**

The framework introduced above can be used to accelerate the execution of quantum algorithms in networks by utilizing the information about the connections. To demonstrate this effect we define a restricted quantum search problem and provide its solution based on the phase estimation algorithm performed locally on the nodes. In this case we obtain quadratic speed-up compared to the quantum search procedure ignoring the phase shifts.

Subsequently we argue that the similar effect can be obtained in more general scenarios, in particular in the case of search on a multilevel network, where the speed-up rate may be exponential.

**Quantum search with prior knowledge**

In this section we consider a search problem where marked node $m$ is to be found with use of the oracle operator that flips the phase of the corresponding state $\ket{m}$ of the position register: $O_m\ket{m} = -\ket{m}$. We assume that it is possible to obtain additional information about the structure during the walk. In order to maintain quadratical speed-up over reduced search space we aim at performing restricted walk harnessing the information encoded in the phase shifts and find the marked node using optimal number of oracle queries.

**Perfect tree case**

A perfect $k$-ary tree is a tree where within each level every node has either 0 or $k$ children and in which all leaf nodes are at the same depth i.e. a tree with constant branching factor.

Let us consider a perfect $k$-ary tree network with $k = 2d$ and depth $L$ with $N = (2d)^L$ leaf nodes. We assume that there are two types of edges: valid and invalid. At each node the possible directions are grouped in $d$ pairs so that within each pair one direction is marked as valid and one as invalid. Thus there are $n = d^L = N \log d / \log 2d$ valid nodes i.e. leaf nodes accessible from the root with valid edges. The example of such setup with $2d = 4$ and $n = \sqrt{N}$ is presented in Figure 1. We assume that one of the valid nodes is marked by the oracle operator. The goal is to perform a walk only on the valid edges and, in result, to reduce the required number of steps.

The proposed search algorithm is based on amplitude amplification [44] as described in Algorithm 1. The crucial part of Algorithm 1 is to perform the spreading part in such a way that one prepares equal superposition of the valid leaves only. The method is presented as Algorithm 2. By combining these pro-
Figure 1: Network based on a perfect k-ary tree of degree $k = 4$. Blue solid, red dashed and black dotted lines represent valid, invalid and unassigned edges respectively. The number of valid nodes (filled blue) is reduced quadratically.

Algorithm 1: Amplitude amplification with the use of a spreading operator $U$ and the number of valid nodes equal to $n$

1. Prepare the initial state $|0\rangle$ at an arbitrary position.
2. Apply operator $U$ to spread on the valid edges.
3. Perform $\left\lceil \frac{\pi}{4} \sqrt{n} \right\rceil$ steps:
   (a) Apply the oracle operator.
   (b) Reverse the spreading with the inverse operator $U^\dagger$.
   (c) Apply operator $1 - 2|0\rangle\langle 0|$.
   (d) Perform the spreading with operator $U$.
4. Measure the position register.

This procedure makes the probability of measuring the marked node is $1/\sqrt{N}$ instead of $1/N$ and the resulting search complexity is $O(\sqrt{N}).$

Corollary 1 For a search problem on a tree network of degree 4 with phase changing edges $\varphi \in \{0, \pi/2\}$ grouped in pairs where half of the edges are valid, Algorithm 1 allows finding the marked vertex in $O(\sqrt{N})$ steps with probability $O(1)$.

Proof of the corollary is a consequence of Amplitude amplification properties and Fact 1.

Theorem 1 (Amplitude amplification [44]) Let $n$ define a reflection operator $R_0$ that flips the phase of the initial state $|0\rangle$ and does not affect any orthogonal state, an oracle operator $O_m$ that flips the phase of the marked state $|m\rangle$ and does not affect any orthogonal state and an spreading operator $A$ such that $|\langle m | A | 0 \rangle|^2 = a$. Suppose $a > 0$, and set $t = \left\lceil \frac{\pi}{4\theta_a \sqrt{n}} \right\rceil$, where $\theta_a$ is defined so that $\sin^2(\theta_a) = a$.
and $0 < \theta_a \leq \pi/2$. Then, if we compute $(A R_0 A^\dagger O_m)^t A |0\rangle$ and measure the system, the outcome is good with probability at least \(\max(1 - a, a)\) and there exists a quantum algorithm that finds a good solution with certainty using a number of applications of $A$ and $A^\dagger$ which is in $\Theta(1/\sqrt{a})$ in the worst case.

Given that the spreading operator $U$ allows one to measure the marked node with probability $1/\sqrt{N}$ the overall computational complexity is $O(\sqrt{N})$. We provide spreading procedure analysis in the next section.

For the purpose of discussing the speed-up, we assume that gaining the information encoded in the phase is not possible a priori i.e. a procedure allowing one to test whether a node is valid is not provided. Thus, the alternative to our approach is a search without the additional knowledge resulting in the search among $N$ labels with quantum computational complexity equal to $O(\sqrt{N})$. The number of steps required for the phase estimation results in a constant factor change in the complexity. As such the search with the prior knowledge provides a quadratic speed-up in the considered case over naive quantum search.

Details of Algorithm

In the following section we consider the spreading operator action.

**Fact 1** After applying the spreading operator $U$ to the initial state the probability of measuring the marked node is equal to $1/n$.

We justify the fact by showing that each step of the spreading walk prepares equal superposition of the valid nodes, and by induction the resulting state is equal superposition of the valid leaves with measurement probability of each of them equal to $1/n$.

We consider a system consisting of three registers: position $\mathcal{X}_p = C^{N(L+1)}$, coin (direction) $\mathcal{X}_c = C^{d+1}$ and memory $\mathcal{X}_m = C^p$. We start in the state

$$ |\psi_0\rangle = |0, 0, 0\rangle \in \mathcal{X}_p \otimes \mathcal{X}_c \otimes \mathcal{X}_m. \quad (7) $$

Let us note that in such system each node has the same number of internal states corresponding to directions. For the root node and the leaves this does not accurately model the tree structure. In order to apply regular graph walk model we assign loops to all of the problematic directions.

At each step we begin by preparing the superposition over possible directions and initializing the memory in the equal superposition of all possible phase label values. This is implemented by an operator $P \in L(\mathcal{X})$ that rotates a state in the initial form $|0, 0\rangle \in \mathcal{X}_c \otimes \mathcal{X}_m$ into $|s\rangle = \sum_c \sum_j |c, j\rangle$ at any position $x$:

$$ P = \sum_x |x\rangle \langle x| \otimes 1_{|0, 0\rangle \rightarrow |s\rangle}. \quad (8) $$
Algorithm 2: Spreading part of Algorithm 1 – operator $U$ – restricted to the valid edges

1. Perform for each of the layers of the network:
   
   (a) Prepare the superposition of directions using the coin operator $P$ given in Eq. (8).
   
   (b) Estimate phase using the operator $E$ from Eq. (4).
   
   (c) Prepare the superposition of valid directions using coin operator $C$ given in Eq. (10).
   
   (d) Apply the shift operator $S$, given in Eq. 2, in order to transfer onto the lower layer with the use of the valid edges.
   
   (e) Reset the superposition getting the initial form of the state with operator $A$ in Eq. (11).

2. Resume the overall algorithm.

Operator $U_{(a)\rightarrow (b)}$ alters only states from $\text{span}(|a\rangle, |b\rangle)$ with operator $|b\rangle \langle a| + |b\prime\rangle \langle a\prime|$. In particular

\[
U_{(a)\rightarrow (b)} |x\rangle = \begin{cases} 
|a\rangle, & |x\rangle \perp \text{span}(|a\rangle, |b\rangle), \\
|b\rangle, & |x\rangle = |a\rangle, \\
|b\prime\rangle, & |x\rangle = |a\prime\rangle,
\end{cases}
\]

where $|a\prime\rangle$ and $|b\prime\rangle$ denote normalized states $|b\rangle - |a\rangle \langle a|b\rangle$ and $|a\rangle - |b\rangle \langle b|a\rangle$ respectively.

Then we perform the phase estimation procedure given in Eq. (4). The algorithm uses the memory register to control the overall phase. After performing the Fourier transform we obtain the value of the phase at the memory register.

Having determined which phase is assigned to which direction we transform equal superposition of all of the directions into a superposition of the valid directions only. Due to the grouping of the directions and phases we can perform this transition with the use of a unitary operator $C \in L(\mathcal{X}_C \otimes \mathcal{X}_M)$ acting on joint coin and memory registers:

\[
C = \frac{1}{\sqrt{2}} \sum_{l=0}^{d-1} |2l, g\rangle \langle g_{2l}^+| + |2l + 1, g\rangle \langle g_{2l+1}^+| + |2l + 1, b\rangle \langle g_{2l+1}^-| + |2d, b\rangle \langle g_{2d}^-|,
\]

where the $g, b$ stand for valid and invalid phase labels. The introduced operator is designed to properly transform a state of a pair $l$ of directions $2l, 2l + 1$ depending on which direction is valid. If direction $2l$ (or $2l + 1$) is valid the state of
the pair is $|g_{2l}^+\rangle = |2l, g\rangle + |2l + 1, b\rangle$ (or $|g_{2l+1}^+\rangle = |2l, b\rangle + |2l + 1, g\rangle$ correspondingly) and is transformed into a valid direction $|2l, g\rangle$ (or $|2l + 1, g\rangle$). One should note that the restriction (directions grouped in pairs) is introduced in order to provide a simple unitary example useful for a search task. For other tasks, such as routing, where the spreading does not have to be reversible, it is possible to implement the direction selection, with more general quantum channel using open walk model, and avoid such limitations [45].

When valid directions are encoded in the coin register we perform the shift operator and then transform resulting states into the initial form with operator

$$A = \sum_x |x\rangle \langle x| \otimes |\uparrow, g\rangle - |0, 0\rangle,$$  \hspace{1cm} \text{(11)}$$

where $\uparrow$ denotes the direction leading to the parent node and $g$ the valid phase label.

As the final result we obtain equal superposition over all leaves that are reachable using only valid edges. This enables us to use procedure described in Algorithm I to execute search on valid nodes only.

**Generalized tree case**

In the example presented above we have restricted ourselves to the situation where only two types of edges are distributed equally in the network layers. However, the presented scheme can be applied to more complicated phase configurations and validation methods. It is important to note that the setting is straightforward to generalize in order to increase the number of edges in the group and in result decrease the factor of valid nodes.

In general if only 2 out of $2^R$ (in general $k$ out of $k^R$) of the edges are valid at each node the number of valid nodes is reduced accordingly: $n = \sqrt[3]{N}$. We obtain search complexity of order $O(\sqrt[3]{N})$, compared to $O((\sqrt[3]{N})^R)$. This class of problems generates arbitrarily large polynomial speed-up. The polynomial degree increases linearly with with exponential growth of the degree of the tree and corresponding valid edges ratio.

The grouping of the edges assumed in the model of unitary selection of the valid edges can be seen as clustering separate dimensions. In such scenario we restrict the walker to move only in one direction within the dimension. Such behaviour commonly occurs in quantum walks. When considering networks with simple representation in the Fourier basis the edges are naturally grouped into classes [46]. A similar approach also frequently appears in scale free networks and other regular graph-based models [14].

**Multilevel network case**

The tree network model discussed in the previous section is suitable to show the basic example in details, but it can only exhibit polynomial complexity speed-
Figure 2: Network based on a multilevel structure. Blue solid and grey dashed lines represent valid and invalid edges respectively. Edges outgoing from invalid nodes are not shown. The number of valid nodes (filled blue) at the bottom level is reduced quadratically.

up rate. In more general cases additional information can cause exponential complexity decay.

The walk model for the multilevel network is analogous to the tree case. The shift operator act as described in eq. (2) taking into account modified connections. Operations on the nodes are local and thus almost the same. Main difference lies in the fact that instead of having one parent node, one need to consider a number of parents and a corresponding state being a superposition of proper directions.

Let us consider a network composed of many layers, such that every layer consists of the same number of nodes \( N \). We assume, that we are able to prepare a state being an equal superposition of all of the nodes from the top layer (e.g. with use of a common root-parent node). Again we assume, that there are 2 pairs of edges outgoing downwards from each of the nodes. Exactly one edge in every pair is valid. An example of valid edges assignment is shown in Fig. 2.

In this case the measure of the problem size is the number of possible outcomes \( N \), which is equal to the number of nodes in the bottom layer. We consider a scheme where the number of valid nodes \( n \) in the last layer is fixed. Thus, layer width \( N \) grows exponentially as \( N = n2^{D-1} \), where \( D \) is network depth (layers number). We are interested in complexity of finding a marked node for fixed number of valid nodes when the number of layers increases. The quantum algorithm is very similar to the previous case and the resulting query complexity is constant for fixed valid nodes set size. The number of required steps in the corresponding algorithm increases logarithmically.

**Model potential**

This examples are designed to show the advantages of including the phase shift in a walk scheme. In described cases obtained speed-up is always quadratical
compared to the classical case where all the information encoded into network is available, thus the speed-up rate is not better than in the standard Grover’s search. However, a convenient way to harness classical heuristics in quantum search is of great interest, because without the method for incorporating the additional knowledge the quantum speed-up gain is lost. The presented model is especially convenient because of the fact that labelling edges in the network with phase shifts does not require any dependence on directions labels. Moreover, using greater number of possible phases one could describe many different edges classes and change its behaviour dynamically with change of the coin operator only. In particular when different edges classes correspond to different heuristics evaluation one can control the threshold that determine active/inactive edges on the run without altering the network structure.

**Concluding remarks**

The aim of this work is to study possibilities of developing the quantum walk model in order to increase its algorithmic potential. In this work we provide the evidence that the model allows one to perform efficient restricted walk propagation on tree-alike structures. Moreover, the restrictions can utilize network structure containing information about the connections without reference to the directions labelling. Additionally, the information may take a form of non-binary evaluation function. The further research will focus on the issue whether the model is suitable for more sophisticated protocols with the use of similar routing scheme. The presented work gives foundations for studying computation methods that allows local determination of network properties and driving the walk behaviour. In particular, the algorithm may be useful in the context of quantum heuristics and mobile agents methods.

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