Invited Paper

Partition of graphs and quantum walk based search algorithms

Yusuke Ide^{1 a)}

¹ School of Knowledge Science, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi 923-1292, Japan

^{a)} ide@jaist.ac.jp

Received August 30, 2018; Revised September 18, 2018; Published January 1, 2019

Abstract: In this paper, we show reduction methods for search algorithms on graphs using quantum walks. By using a graph partitioning method called equitable partition for the the given graph, we determine “effective subspace” for the search algorithm to reduce the size of the problem. We introduce the equitable partition for quantum walk based search algorithms and show how to determine “effective subspace” and reduced operator.

Key Words: quantum walks, quantum search, equitable partition

1. Introduction

In the last two decades, the study of the quantum walks (QWs) has been extensively developed by many researchers. QWs can be viewed as quantum counterparts of usual random walks (RWs) but they have several different features from that of RWs. For example, if we consider the discrete-time QW on the one-dimensional lattice case with parameters corresponding to the simple RW, the position X_n of the walker at time n follows the following limit theorem [15, 16]:

$$\frac{X_n}{n} \Rightarrow Z \quad (n \rightarrow \infty).$$

Here the random variable Z has the following probability density function:

$$f(x) = \begin{cases} \frac{1}{\pi(1-x^2)\sqrt{1-2x^2}}, & \text{if } -1/\sqrt{2} < x < 1/\sqrt{2}, \\ 0, & \text{otherwise.} \end{cases}$$

Note that $\Rightarrow$ stands for the weak convergence. Let $\mathbb{E}_n$ be the expectation with respect to the probability distribution of X_n for each $n = 0, 1, \dots$. We also consider the characteristic function $\phi_n(\xi) = \mathbb{E}_n[\exp(i\xi X_n/n)]$ of X_n/n for each $\xi \in \mathbb{R}$ where i (resp. $\mathbb{R}$) denotes the imaginary unit (resp. the set of real numbers). Then $X_n/n \Rightarrow Z$ is equivalent to $\lim_{n \rightarrow \infty} \phi_n(\xi) = \int_{-\infty}^{\infty} e^{i\xi x} f(x) dx$ for all $\xi \in \mathbb{R}$.

This theorem corresponds to the central limit theorem for the RWs. The theorem shows that the position of the quantum walker spreads in ballistic order (order n) not in diffusive order (order $\sqrt{n}$) of the random walker. The limit distribution (Fig. 1) is also different from the Gaussian distribution which is appear in the central limit theorem for the RWs (Fig. 2).

Fig. 1. Limit distribution for discrete-time QWs.

Fig. 2. Limit distribution for RWs.

Recently, QWs have received much attention in various fields not only mathematical interests but also such as experimental realization [11, 22], connection between topological phase [3, 14], reduction method for radioactivity [9, 20], quantum search algorithms [1, 2, 4–7, 18, 23]. There are good review articles for the theory of QWs such as [12, 13, 17, 19, 21, 24].

In this paper, we show reduction methods for search algorithms on graphs using QWs. By using the equitable partition [8] for the graph, we determine “effective subspace” for the search algorithm to reduce the size of the problem. For this purpose, we review two types of QWs, discrete-time and continuous-time versions, in Sec. 2. In Sec. 3, we introduce QW based search algorithms. The main contribution of this paper is Sec. 4. In this section, we introduce the equitable partition for QW based search algorithms and show how to determine “effective subspace” and reduced operator.

2. Quantum walks

2.1 Discrete-time quantum walk (DTQW)

Let $G = (V(G), E(G))$ be a simple graph (undirected graph without self-loops and multiple edges) with its vertex set $V(G) = \{0, 1, \dots, N-1\}$ and edge set $E(G) \subset V(G) \times V(G)$. As an example, for the complete graph on N vertices K_N which is the simple graph with $\binom{N}{2}$ edges (fully connected), the edge set is defined by $E(K_N) = \{(j, k) : 0 \leq j < k \leq N-1\}$. More concretely, for K_4 and K_5 (Fig. 3), the edge sets are defined by $E(K_4) = \{(0, 1), (0, 2), (0, 3), (1, 2), (1, 3), (2, 3)\}$ and $E(K_5) = \{(0, 1), (0, 2), (0, 3), (0, 4), (1, 2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4)\}$.

Discrete-time quantum walk (DTQW) is a quantum dynamics on the graph with the following Hilbert space $\mathcal{H}_{DTQW}$:

$$\mathcal{H}_{DTQW} = \text{Span} \{ |j\rangle \otimes |k\rangle, |k\rangle \otimes |j\rangle : (j, k) \in E(G) \},$$

where $|j\rangle = {}^T[0, \dots, 0, \overbrace{1}^{j\text{-th}}, 0, \dots, 0]$ is the N -dimensional standard basis (column vector, ${}^T A$ denotes the transpose of A) corresponding to the vertex j and $|j\rangle \otimes |k\rangle$ represents the tensor product of

Fig. 3. The complete graphs K_4 and K_5 .

the two bases $|j\rangle$ and $|k\rangle$. The Hilbert space $\mathcal{H}_{DTQW}$ is the Hilbert space spanned by the basis $\{|j\rangle \otimes |k\rangle, |k\rangle \otimes |j\rangle : (j, k) \in E(G)\}$. We usually call each element in the Hilbert space as state. The state $|j\rangle \otimes |k\rangle$ is interpreted as “the state (direction) from the vertex j to an adjacent vertex k ” (Fig. 4).

Fig. 4. The state $|j\rangle \otimes |k\rangle$.

There are many choices of the definition of the time evolution operator (unitary matrix) U of DTQW on the graph G . Here we adopt the following definition:

$$U = SC.$$

Where S is called the flip-flop type shift operator which governs the motion of the walker. The definition of the shift is the following (Fig. 5):

$$S(|j\rangle \otimes |k\rangle) = |k\rangle \otimes |j\rangle, \text{ for } (j, k) \in E(G).$$

Fig. 5. Flip-flop type shift.

Also C is called the coin operator which mixes the walker’s states. The coin operator is given by

$$C = \sum_{j \in V(G)} |j\rangle \langle j| \otimes C_j,$$

where $\langle j|$ is the conjugate transpose of $|j\rangle$. The unitary matrix C_j is a d_j ($=$ the degree of the vertex j , i.e., the number of edges connected with the vertex j) -dimensional unitary matrix which is defined by

$$C_j |k\rangle = \sum_{(j, k') \in E(G)} (C_j)_{k', k} |k'\rangle,$$

for each k with $(j, k) \in E(G)$. From the definition of the coin operator C , we can see that

$$C|j\rangle \otimes |k\rangle = \left(\sum_{j \in V(G)} |j\rangle \langle j| \otimes C_j \right) |j\rangle \otimes |k\rangle = |j\rangle \otimes C_j |k\rangle = \sum_{(j, k') \in E(G)} (C_j)_{k', k} |j\rangle \otimes |k'\rangle,$$

for each $(j, k) \in E(G)$. From this observation, we can say that the coin operator C “mixes” each state corresponding to each vertex $j \in V(G)$ with suitable weights (Fig. 6).

Fig. 6. Action of the coin operator on the state $|j\rangle \otimes |k\rangle$.

There are many choices of C_j . One of a typical choice of C_j is the following Grover's coin $U_G(j)$ which corresponds to the simple random walk on G :

$$U_G(j) = 2|D_j\rangle\langle D_j| - I_{d_j},$$

where $|D_j\rangle$ is called the diagonal state corresponding to the vertex j which is defined by

$$|D_j\rangle = \frac{1}{\sqrt{d_j}} \sum_{(j,k) \in E(G)} |k\rangle,$$

and I_k denotes the identity matrix of order k .

For DTQW, we choose a unit vector (initial state) $|\Psi_{N,0}\rangle \in \mathcal{H}_{DTQW}$ of the walker. Then we consider the time evolution

$$|\Psi_{N,n}\rangle = U^n |\Psi_{N,0}\rangle,$$

for $n = 0, 1, \dots$. Here $|\Psi_{N,n}\rangle$ is called the probability amplitude at time n . Using this probability amplitude, we define the probability

$$\mathbb{P}_{N,n}(s) = \|(|s\rangle\langle s| \otimes I_{d_s}) |\Psi_{N,n}\rangle\|^2,$$

that the walker is found on $s \in V(G)$ at time n .

2.2 Continuous-time quantum walk (CTQW)

Again we consider a simple graph $G = (V(G), E(G))$ with $V(G) = \{0, 1, \dots, N-1\}$. Continuous-time quantum walk (CTQW) is a quantum dynamics on the graph with the following Hilbert space $\mathcal{H}_{CTQW}$ (Fig. 7):

$$\mathcal{H}_{CTQW} = \text{Span}\{|j\rangle : j \in V(G)\}.$$

On this Hilbert space $\mathcal{H}_{CTQW}$, we define the time evolution operator of CTQW. We choose an N -dimensional Hermitian matrix M_G with $(M_G)_{j,k} \neq 0$ when $(j,k) \in E(G)$ and $(M_G)_{j,k} = 0$ when $(j,k) \notin E(G)$. The component $(M_G)_{j,k}$ is interpreted as “the weight of the edge $(j,k) \in E(G)$ ” as Fig. 8.

Fig. 7. The basis of $\mathcal{H}_{CTQW}$.

Fig. 8. The weight of the edge $(j,k) \in E(G)$.

For the time $t \geq 0$, we define the time evolution operator

$$U_{M_G}(t) = \exp(itM_G) = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} M_G^k,$$

of CTQW on G corresponding to M_G . We note that CTQW is nothing but quantum dynamics determined by the Schrödinger equation with its Hamiltonian M_G . We choose a unit vector (initial state) $|\Psi_{N,0}\rangle \in \mathcal{H}_{CTQW}$ then the time evolution

$$|\Psi_{N,t}\rangle = U_{M_G}(t)|\Psi_{N,0}\rangle,$$

for $t \geq 0$ is defined. Here $|\Psi_{N,t}\rangle$ represents the probability amplitude at time t . We define the probability that the walker is found on $s \in V(G)$ at time t as

$$\mathbb{P}_{N,t}(s) = |\langle s | \Psi_{N,t} \rangle|^2.$$

One of a typical choice of M_G is the adjacency matrix

$$(A_G)_{j,k} = \begin{cases} 1 & \text{if } (j,k) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

of the graph G .

For example, we show the time evolution for $G = K_2$ the complete graph on 2 vertices case. In this case,

$$A_{K_2} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Thus we have

$$A_{K_2}^{2k} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad A_{K_2}^{2k+1} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Therefore we obtain

$$\begin{aligned} U_{A_{K_2}}(t) &= \exp(itA_{K_2}) = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} A_{K_2}^k \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k)!} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)!} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} \cos t & i \sin t \\ i \sin t & \cos t \end{bmatrix}. \end{aligned}$$

If we consider the initial state as $|\Psi_{n,0}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ which is corresponding to the case that the walker starts from the vertex $0 \in V(K_2)$ then we can calculate

$$|\Psi_{N,t}\rangle = U_{A_{K_2}}(t)|\Psi_{n,0}\rangle = \begin{bmatrix} \cos t & i \sin t \\ i \sin t & \cos t \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos t \\ i \sin t \end{bmatrix}.$$

Therefore we obtain

$$\begin{aligned} \mathbb{P}_{N,t}(0) &= |\langle 0 | \Psi_{N,t} \rangle|^2 = |\cos t|^2 = \cos^2 t, \\ \mathbb{P}_{N,t}(1) &= |\langle 1 | \Psi_{N,t} \rangle|^2 = |i \sin t|^2 = \sin^2 t. \end{aligned}$$

3. Quantum walk based search algorithms

3.1 DTQW cases

In this section, we consider discrete-time quantum walk based search (DTQW search) on simple graph $G = (V(G), E(G))$ with $V(G) = \{0, 1, \dots, N-1\}$. Let $w \in V(G)$ be the vertex which we want to find (marked vertex). For DTQW search, we use the following special coin operator:

$$C_j = \begin{cases} -I_{d_w}, & \text{if } j = w, \\ U_G(j), & \text{otherwise.} \end{cases}$$

Then we consider the DTQW on G with the uniform initial state

$$|\Psi_0\rangle = \frac{1}{\sqrt{2|E(G)|}} \sum_{j=0}^{N-1} \sum_{(j,k) \in E(G)} |j\rangle \otimes |k\rangle.$$

The main task for DTQW search is finding a time $T = \mathcal{O}(\sqrt{N})$ such that we can attain

$$\mathbb{P}_{N,T}(w) \approx 1 \quad (N \rightarrow \infty).$$

For example, for DTQW search on the hypercube case, there is a time $T = \mathcal{O}(\sqrt{N})$ such that the search is successful [23]. For the square lattice cases [2], there also exist times $T = \mathcal{O}(\sqrt{N})$.

3.2 CTQW cases

In this section, we consider continuous-time quantum walk based search (CTQW search) on simple graph $G = (V(G), E(G))$ with $V(G) = \{0, 1, \dots, N-1\}$. The Hermitian matrix H_G for CTQW search on G is defined by

$$H_G = |w\rangle\langle w| + \gamma A_G \quad (\gamma \in \mathbb{R}),$$

where $w \in V(G)$ is the marked vertex. Now we consider the CTQW on G with its time evolution operator U_{H_G} . The main task for CTQW search is finding a suitable $\gamma \in \mathbb{R}$ and a time $T = \mathcal{O}(\sqrt{N})$ such that we can attain

$$\mathbb{P}_{N,T}(w) \approx 1 \quad (N \rightarrow \infty),$$

with the uniform initial state

$$|\Psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |j\rangle.$$

For example, CTQW search on the complete graph, the hypercube and the square lattice cases, there exist suitable $\gamma \in \mathbb{R}$ and a time $T = \mathcal{O}(\sqrt{N})$ such that the search are successful [7]. For the Erdős-Rényi random graph with suitable condition for the connection probability cases, there also exist suitable $\gamma \in \mathbb{R}$ and a time $T = \mathcal{O}(\sqrt{N})$ such that the search are successful for almost all generated graphs [4].

4. Equitable partition and quantum walk search

4.1 Equitable partition of graphs for quantum walk search

For both DTQW search and CTQW search, a partition of the graph so-called equitable partition [8] is very useful. Note that the equitable partition can be viewed as a generalization of the modular partition [10]. Without loss of generality, we assume that the marked vertex is $0 \in V(G)$. We consider the partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\bar{J-1}})$ of $G = (V(G), E(G))$ which is satisfied the following 3 conditions:

1. $V(G_{\bar{0}}) = \{0\}$.
2. $V(G) = \bigcup_{\bar{j}=0}^{J-1} V(G_{\bar{j}})$, $V(G_{\bar{j}}) \cap V(G_{\bar{k}}) = \emptyset$ ($\bar{j} \neq \bar{k}$).

3. For each $\bar{0} \leq \bar{j}, \bar{k} \leq \bar{J}-1$, there exists a non-negative integer $d_{\bar{j}, \bar{k}}$ such that $d_{\bar{j}, \bar{k}} = |\{w \in V(G_{\bar{k}}) : (v, w) \in E(G)\}|$ for each $v \in V(G_{\bar{j}})$.

This partition is a special case of so-called equitable partition. We use the notation $G_{\bar{j}} \sim G_{\bar{k}}$ if $d_{\bar{j}, \bar{k}} \neq 0$.

The partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\bar{J}-1})$ of $G = (V(G), E(G))$ consists of $\bar{J}$ subgraphs. For each subgraph $G_{\bar{j}}$ is $d_{\bar{j}, \bar{j}}$ -regular graph. Especially, $G_{\bar{0}}$ is the null graph ($d_{\bar{0}, \bar{0}} = 0$) which consists of only the marked vertex $0 \in V(G)$. In addition, for each vertex $v \in V(G_{\bar{j}})$ the number of edges connected to the vertices in $V(G_{\bar{k}})$ is $d_{\bar{j}, \bar{k}}$ regardless the choice of vertex. In Fig. 9, we show an example of the partition. In this case, $V(G_{\bar{0}}) = \{0\}$, $V(G_{\bar{1}}) = \{1, 4\}$, $V(G_{\bar{2}}) = \{2, 3\}$ and $d_{\bar{0}, \bar{0}} = 0$, $d_{\bar{0}, \bar{1}} = 2$, $d_{\bar{0}, \bar{2}} = 0$, $d_{\bar{1}, \bar{0}} = 1$, $d_{\bar{1}, \bar{1}} = 0$, $d_{\bar{1}, \bar{2}} = 2$, $d_{\bar{2}, \bar{0}} = 0$, $d_{\bar{2}, \bar{1}} = 2$, $d_{\bar{2}, \bar{2}} = 1$. By using this partition, we can construct efficient eigenspace for both DTQW search and CTQW search. Note that for each graph G , the graph itself, i.e., $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\bar{N}-1})$ with $V(G_{\bar{j}}) = \{j\}$ for each $j \in V(G)$, is a trivial equitable partition. Therefore the proposed method works well for graphs with equitable partition consists of small numbers of subgraphs.

Fig. 9. Partition of the graph G .

4.2 DTQW cases

In this section, we consider DTQWs defined by “Grover type coins” on simple, connected graphs. For each $j \in V(G)$, we consider the following coin:

$$C_j = (\lambda_{j,1} - \lambda_{j,2})|D_j\rangle\langle D_j| + \lambda_{j,2}I_{d_j},$$

where $\lambda_{j,1}, \lambda_{j,2} \in \mathbb{C}$ with $|\lambda_{j,1}| = |\lambda_{j,2}| = 1$. Note that if $\lambda_{j,1} \neq \lambda_{j,2}$ then this Grover type coin C_j has two eigenvalues $\lambda_{j,1}$ and $\lambda_{j,2}$ with multiplicities 1 and $N-1$, respectively.

Here we consider the equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\bar{J}-1})$ with $n_{\bar{j}} = |V(G_{\bar{j}})|$ of G . We define the following uniform states related to the partition:

$$|\bar{j}\bar{k}\rangle = \begin{cases} \frac{1}{\sqrt{n_{\bar{j}}d_{\bar{j}, \bar{k}}}} \sum_{\substack{j \in V(G_{\bar{j}}), k \in V(G_{\bar{k}}), \\ (j,k) \in E(G)}} |j\rangle \otimes |k\rangle, & \text{if } G_{\bar{j}} \sim G_{\bar{k}}, \\ \mathbf{0}, & \text{otherwise,} \end{cases}$$

for each $\bar{0} \leq \bar{j}, \bar{k} \leq \bar{J}-1$ where $\mathbf{0}$ is the zero vector of $\mathcal{H}_{DTQW}$. The state $|\bar{j}\bar{k}\rangle$ is the uniform state on the states corresponding to edges from $G_{\bar{j}}$ to $G_{\bar{k}}$. Assume that every vertices in $G_{\bar{j}}$ have the same coin $C_{\bar{j}}$ for $\bar{0} \leq \bar{j} \leq \bar{J}-1$ then we obtain

$$\begin{aligned} C|\bar{j}\bar{k}\rangle &= \frac{\lambda_{\bar{j},1} - \lambda_{\bar{j},2}}{d_{\bar{j}}} \sqrt{\frac{d_{\bar{j}, \bar{k}}}{n_{\bar{j}}}} \left(\sum_{G_{\bar{j}} \sim G_{\bar{k}'}} \sqrt{n_{\bar{j}}d_{\bar{j}, \bar{k}'}} |\bar{j}\bar{k}'\rangle \right) + \lambda_{\bar{j},2} |\bar{j}\bar{k}\rangle \\ &= \frac{\lambda_{\bar{j},1} - \lambda_{\bar{j},2}}{d_{\bar{j}}} \left(\sum_{G_{\bar{j}} \sim G_{\bar{k}'}} \sqrt{d_{\bar{j}, \bar{k}}d_{\bar{j}, \bar{k}'}} |\bar{j}\bar{k}'\rangle \right) + \lambda_{\bar{j},2} |\bar{j}\bar{k}\rangle, \end{aligned}$$

with convention $G_{\bar{j}} \sim G_{\bar{j}}$ for $\bar{0} \leq \bar{j} \leq \overline{J-1}$. On the other hand,

$$\begin{aligned} S|\bar{j}\bar{k}\rangle &= S \left(\frac{1}{\sqrt{n_{\bar{j}}d_{\bar{j},\bar{k}}}} \sum_{\substack{j \in V(G_{\bar{j}}), k \in V(G_{\bar{k}}), \\ (j,k) \in E(G)}} |j\rangle \otimes |k\rangle \right) = \frac{\sqrt{n_{\bar{k}}d_{\bar{k},\bar{j}}}}{\sqrt{n_{\bar{j}}d_{\bar{j},\bar{k}}}} \frac{1}{\sqrt{n_{\bar{k}}d_{\bar{k},\bar{j}}}} \sum_{\substack{k \in V(G_{\bar{k}}), j \in V(G_{\bar{j}}), \\ (k,j) \in E(G)}} |k\rangle \otimes |j\rangle \\ &= |\bar{k}\bar{j}\rangle, \end{aligned}$$

where we use the relations $(j, k) \in E(G)$ then $(k, j) \in E(G)$ and $n_{\bar{j}}d_{\bar{j},\bar{k}} = n_{\bar{k}}d_{\bar{k},\bar{j}}$ coming from simplicity of the graph. This shows that the action of $U = SC$ is

$$U|\bar{j}\bar{k}\rangle = \frac{\lambda_{\bar{j},1} - \lambda_{\bar{j},2}}{d_{\bar{j}}} \left(\sum_{G_{\bar{j}} \sim G_{\bar{k}'}} \sqrt{d_{\bar{j},\bar{k}}d_{\bar{j},\bar{k}'}} |\bar{k}'\bar{j}\rangle \right) + \lambda_{\bar{j},2} |\bar{k}\bar{j}\rangle,$$

for $\bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}$.

From this observation, the action of the time evolution operator $U = SC$ is closed on the subspace $\text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$ of $\mathcal{H}_{DTQW}$. Also the uniform initial state $|\Psi_0\rangle$ is represented by linear combination of uniform states related to the partition,

$$|\Psi_0\rangle = \frac{1}{\sqrt{2|E(G)|}} \sum_{j=0}^{N-1} \sum_{(j,k) \in E(G)} |j\rangle \otimes |k\rangle = \frac{1}{\sqrt{2|E(G)|}} \sum_{\bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}} \sqrt{n_{\bar{j}}d_{\bar{j},\bar{k}}} |\bar{j}\bar{k}\rangle.$$

This shows that $|\Psi_0\rangle \in \text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$. We summarize this fact as the following proposition:

Proposition 4.1 Consider the DTQW defined by Grover type coin with the equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\overline{J-1}})$ starting from the uniform initial state $|\Psi_0\rangle$. Then we have $|\Psi_0\rangle \in \text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$. Assume that every vertices in $G_{\bar{j}}$ have the same coin $C_{\bar{j}}$. Then the action of the time evolution operator $U = SC$ is closed on the subspace $\text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$ of $\mathcal{H}_{DTQW}$ as follows:

$$U|\bar{j}\bar{k}\rangle = \frac{\lambda_{\bar{j},1} - \lambda_{\bar{j},2}}{d_{\bar{j}}} \left(\sum_{G_{\bar{j}} \sim G_{\bar{k}'}} \sqrt{d_{\bar{j},\bar{k}}d_{\bar{j},\bar{k}'}} |\bar{k}'\bar{j}\rangle \right) + \lambda_{\bar{j},2} |\bar{k}\bar{j}\rangle, \quad (1)$$

for $\bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}$.

Proposition 4.1 states a reduction method for the DTQW defined by Grover type coin with the equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\overline{J-1}})$ starting from the uniform initial state $|\Psi_0\rangle$. Whenever we start from the uniform initial state $|\Psi_0\rangle$, we can only consider the action of the time evolution operator $U = SC$ on $\text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$ that is defined as Eq. (1). This means that we can only consider at most J^2 dimensional subspace of $\mathcal{H}_{DTQW}$ which dimension is $2|E(G)|$. Applying Proposition 4.1 to DTQW search, we have the following theorem:

Theorem 4.2 Consider the DTQW search on simple, connected graph G with the equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\overline{J-1}})$. Then we have $|\Psi_0\rangle \in \text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$. Then the action of the time evolution operator $U = SC$ is closed on the subspace $\text{Span}\{|\bar{j}\bar{k}\rangle : \bar{0} \leq \bar{j}, \bar{k} \leq \overline{J-1}\}$ of $\mathcal{H}_{DTQW}$ as follows:

$$U|\bar{j}\bar{k}\rangle = \begin{cases} \frac{2}{d_{\bar{j}}} \left(\sum_{G_{\bar{j}} \sim G_{\bar{k}'}} \sqrt{d_{\bar{j},\bar{k}}d_{\bar{j},\bar{k}'}} |\bar{k}'\bar{j}\rangle \right) - |\bar{k}\bar{j}\rangle, & \text{if } \bar{j} \neq \bar{0} \text{ and } \bar{0} \leq \bar{k} \leq \overline{J-1}, \\ -|\bar{k}\bar{0}\rangle, & \text{if } \bar{j} = \bar{0} \text{ and } \bar{0} \leq \bar{k} \leq \overline{J-1}. \end{cases}$$

4.3 CTQW cases

In this section, we consider the CTQW search on simple, connected graph G with equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\overline{J-1}})$ with $n_{\bar{j}} = |V(G_{\bar{j}})|$ of G . We define the following uniform states related to the partition:

$$|\bar{j}\rangle = \frac{1}{\sqrt{n_{\bar{j}}}} \sum_{j \in V(G_{\bar{j}})} |j\rangle,$$

for $0 \leq \bar{j} \leq J-1$. By direct calculation, we obtain

$$\begin{aligned} A_G |\bar{j}\rangle &= d_{\bar{j}\bar{j}} |\bar{j}\rangle + \sum_{G_{\bar{j}} \sim G_{\bar{k}}} d_{\bar{k}\bar{j}} \sqrt{\frac{n_{\bar{k}}}{n_{\bar{j}}}} |\bar{k}\rangle = d_{\bar{j}\bar{j}} |\bar{j}\rangle + \sum_{G_{\bar{j}} \sim G_{\bar{k}}} \sqrt{d_{\bar{k}\bar{j}}} \sqrt{\frac{n_{\bar{j}} d_{\bar{j}\bar{k}}}{n_{\bar{j}}}} |\bar{k}\rangle \\ &= d_{\bar{j}\bar{j}} |\bar{j}\rangle + \sum_{G_{\bar{j}} \sim G_{\bar{k}}} \sqrt{d_{\bar{j}\bar{k}} d_{\bar{k}\bar{j}}} |\bar{k}\rangle, \\ &= \sum_{\bar{0} \leq \bar{k} \leq \overline{J-1}} \sqrt{d_{\bar{j}\bar{k}} d_{\bar{k}\bar{j}}} |\bar{k}\rangle, \end{aligned}$$

where we use the relation $n_{\bar{j}} d_{\bar{j}\bar{k}} = n_{\bar{k}} d_{\bar{k}\bar{j}}$ coming from simplicity of the graph.

Now we define a $J \times J$ matrix $\bar{A}_G$ as

$$(\bar{A}_G)_{\bar{j}, \bar{k}} = \sqrt{d_{\bar{j}\bar{k}} d_{\bar{k}\bar{j}}}.$$

Recall that the Hermitian matrix for DTQW search is defined by $H_G = |0\rangle\langle 0| + \gamma A_G$. If we define a $J \times J$ matrix $\bar{H}_G$ as

$$\bar{H}_G = \text{diag}(1, 0, \dots, 0) + \gamma \bar{A}_G,$$

then the action of the Hermitian matrix H_G is closed on the subspace $\text{Span}\{|\bar{j}\rangle : \bar{0} \leq \bar{j} \leq \overline{J-1}\}$ as

$$H_G |\bar{j}\rangle = \bar{H}_G |\bar{j}\rangle,$$

for $\bar{0} \leq \bar{j} \leq \overline{J-1}$. We also obtain $|\Psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{\bar{j}=\bar{0}}^{\overline{J-1}} \sqrt{n_{\bar{j}}} |\bar{j}\rangle \in \text{Span}\{|\bar{j}\rangle : \bar{0} \leq \bar{j} \leq \overline{J-1}\}$. This shows that

$$H(G) |\Psi_0\rangle = \bar{H}_G \left(\frac{1}{\sqrt{N}} \sum_{\bar{j}=\bar{0}}^{\overline{J-1}} \sqrt{n_{\bar{j}}} |\bar{j}\rangle \right),$$

thus

$$\exp(itH(G)) |\Psi_0\rangle = \exp(it\bar{H}_G) \left(\frac{1}{\sqrt{N}} \sum_{\bar{j}=\bar{0}}^{\overline{J-1}} \sqrt{n_{\bar{j}}} |\bar{j}\rangle \right).$$

We summarize this fact as the following theorem:

Theorem 4.3 Consider the CTQW search on simple, connected graph G with the equitable partition $(G_{\bar{0}}, G_{\bar{1}}, \dots, G_{\overline{J-1}})$. Then we have $|\Psi_0\rangle \in \text{Span}\{|\bar{j}\rangle : \bar{0} \leq \bar{j} \leq \overline{J-1}\}$. Define a $J \times J$ matrix $\bar{H}_G$ as

$$\bar{H}_G = \text{diag}(1, 0, \dots, 0) + \gamma \bar{A}_G,$$

where $\bar{A}_G$ is also $J \times J$ matrix with $(\bar{A}_G)_{\bar{j}, \bar{k}} = \sqrt{d_{\bar{j}\bar{k}} d_{\bar{k}\bar{j}}}$. Then the finding probability $\mathbb{P}_{N,t}(0)$ of the marked vertex $0 \in V(G)$ at time t is

$$\mathbb{P}_{N,t}(0) = \left| \langle \bar{0} | \exp(it\bar{H}_G) \left(\frac{1}{\sqrt{N}} \sum_{\bar{j}=\bar{0}}^{\overline{J-1}} \sqrt{n_{\bar{j}}} |\bar{j}\rangle \right) \right|^2.$$

By using Theorem 4.3, we obtain the following concrete example of CTQW search:

Proposition 4.4 Let G be the graph with marked vertex $0 \in V(G)$ which is connected to all the vertices of a d -regular graph with $N - 1$ vertices then we obtain

$$\mathbb{P}_{N,t}(0) = \left(1 - \frac{1}{N}\right) - \left(1 - \frac{2}{N}\right) \cos^2 \left(\frac{\sqrt{N-1}}{d} t \right),$$

when we take $\gamma = 1/d$. Particularly, if we take $T = (d\pi/2)/\sqrt{N-1}$ then we have $\mathbb{P}_{N,T}(0) = 1 - 1/N$. The finding probability $\mathbb{P}_{N,t}(0)$ takes any values in $[1/N, 1 - 1/N]$ with period $2T$.

Proposition 4.4 shows that if we consider a graph with $d = \mathcal{O}(N)$ such that the complete graph K_N then $T = \mathcal{O}(\sqrt{N})$ with $\gamma = \mathcal{O}(1/N)$. In this case, the reduced matrix $\bar{H}_G$ is a 2×2 matrix (simplest case). Finding concrete examples which reduced matrix $\bar{H}_G$ is a general $J \times J$ matrix and the search is successful might be an interesting future problem.

Proof of Proposition 4.4.

In this case, we can consider an equitable partition (G_0, G_1) with $V(G_0) = \{0\}$, $V(G_1) = \{1, \dots, N-1\}$ and $d_{0,0} = 0$, $d_{0,1} = N-1$, $d_{1,0} = 1$, $d_{1,1} = d$. By Theorem 4.3 we have the reduced matrix

$$\bar{H}_G = \begin{bmatrix} 1 & \gamma\sqrt{N-1} \\ \gamma\sqrt{N-1} & \gamma d \end{bmatrix}.$$

In order to obtain eigenvalues and eigenvectors of $\bar{H}_G$, we deal with the following equation:

$$\bar{H}_G (\alpha|\bar{0}\rangle + \beta|\bar{1}\rangle) = \lambda (\alpha|\bar{0}\rangle + \beta|\bar{1}\rangle).$$

This equation is equivalent to

$$\begin{bmatrix} 1 & \gamma\sqrt{N-1} \\ \gamma\sqrt{N-1} & \gamma d \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \lambda \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

If we set $\gamma = 1/d$ then the eigenvalues and eigenvectors $\bar{H}_G|v_{\pm}\rangle = \lambda_{\pm}|v_{\pm}\rangle$ are obtained by

$$\begin{aligned} \lambda_{\pm} &= 1 \pm \frac{\sqrt{N-1}}{d}, \\ |v_{\pm}\rangle &= \frac{|\bar{0}\rangle \pm |\bar{1}\rangle}{\sqrt{2}}. \end{aligned}$$

Therefore we obtain spectral decomposition

$$\exp(it\bar{H}_G) = e^{it\lambda_+}|v_+\rangle\langle v_+| + e^{it\lambda_-}|v_-\rangle\langle v_-|.$$

On the other hand,

$$\begin{aligned} \langle v_{\pm}| \left\{ \frac{1}{\sqrt{N}} (|\bar{0}\rangle + \sqrt{N-1}|\bar{1}\rangle) \right\} &= \frac{1}{\sqrt{2N}} (1 \pm \sqrt{N-1}), \\ \langle \bar{0}|v_{\pm}\rangle &= \frac{1}{\sqrt{2}}. \end{aligned}$$

Then we have

$$\begin{aligned} \langle \bar{0}| \exp(it\bar{H}_G) \left\{ \frac{1}{\sqrt{N}} (|\bar{0}\rangle + \sqrt{N-1}|\bar{1}\rangle) \right\} \\ = e^{it} \left\{ \frac{1}{\sqrt{N}} \cos\left(\frac{\sqrt{N-1}}{d}t\right) + i\sqrt{\frac{N-1}{N}} \sin\left(\frac{\sqrt{N-1}}{d}t\right) \right\}. \end{aligned}$$

As a consequence, we obtain

$$\left| \langle \bar{0}| \exp(it\bar{H}_G) \left\{ \frac{1}{\sqrt{N}} (|\bar{0}\rangle + \sqrt{N-1}|\bar{1}\rangle) \right\} \right|^2 = \left(1 - \frac{1}{N}\right) - \left(1 - \frac{2}{N}\right) \cos^2 \left(\frac{\sqrt{N-1}}{d} t \right).$$

□

5. Summary

In this paper, we show reduction methods for search algorithms on graphs using QWs. By using the equitable partition for the graph, we determine “effective subspace” for the search algorithm to reduce the size of the problem in both DTQW search and CTQW search. It can be an interesting future problem that determining conditions of equitable partition which induce successful DTQW search and CTQW search.

Acknowledgments

The author was supported by the Grant-in-Aid for Young Scientists (B) of Japan Society for the Promotion of Science (Grant No. 16K17652).

References

- [1] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, “One-dimensional quantum walks,” *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, pp. 37–49, 2001.
- [2] A. Ambainis, J. Kempe, and A. Rivosh, “Coins make quantum walks faster,” *Proceedings of the 16th ACM-SIAM Symposium on Discrete Algorithms*, pp. 1099–1108, 2005.
- [3] J.K. Asboth and J.M. Edge, “Edge-state-enhanced transport in a two-dimensional quantum walk,” *Phys. Rev.*, vol. A 91, 022324, 2015.
- [4] S. Chakraborty, L. Novo, A. Ambainis, and Y. Omar, “Spatial search by quantum walk is optimal for almost all graphs,” *Phys. Rev. Lett.*, vol. 116, 100501, 2016.
- [5] A.M. Childs, “Universal computation by quantum walk,” *Phys. Rev. Lett.*, vol. 102, 180501, 2009.
- [6] A.M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D.A. Spielman, “Exponential algorithmic speedup by quantum walk,” *Proceedings of the 35th Annual ACM Symposium on Theory of Computing*, pp. 59–68, 2003.
- [7] A.M. Childs and J. Goldstone, “Spatial search by quantum walk,” *Phys. Rev.*, vol. A 70, 022314, 2004.
- [8] C. Godsil and G.F. Royle, *Algebraic Graph Theory*. Springer-Verlag, New York, 2001.
- [9] A. Ichihara, L. Matsuoka, Y. Kurosaki, and K. Yokoyama, “An analytic formula for describing the transient rotational dynamics of diatomic molecules in an optical frequency comb,” *Chin. J. Phys.*, vol. 51, pp. 1230–1240, 2013.
- [10] M. Habib and C. Paul, “A survey of the algorithmic aspects of modular decomposition,” *Computer Sci. Review*, vol. 4, pp. 41–59, 2010.
- [11] M. Karski, L. Förster, J.-M. Choi, A. Steffen, W. Alt, D. Meschede, and A. Widera, “Quantum walk in position space with single optically trapped atoms,” *Science*, vol. 325, 174, 2009.
- [12] J. Kempe, “Quantum random walks - an introductory overview,” *Contemporary Physics*, vol. 44, pp. 307–327, 2003.
- [13] V. Kendon, “Decoherence in quantum walks - a review. Math. Struct,” *Comp. Sci.*, vol. 17, pp. 1169–1220, 2007.
- [14] T. Kitagawa, M.S. Rudner, E. Berg, and E. Demler, “Exploring topological phases with quantum walks,” *Phys. Rev.*, vol. A 82, 033429, 2010.
- [15] N. Konno, “Quantum random walks in one dimension. Quant,” *Inform. Process*, vol. 1, pp. 345–354, 2002.
- [16] N. Konno, “A new type of limit theorems for the one-dimensional quantum random walk,” *J. Math. Soc. Jpn.*, vol. 57, pp. 1179–1195, 2005.
- [17] N. Konno, “Quantum Walks,” In: *Quantum Potential Theory*, U. Franz and M. Schürmann, Eds., *Lecture Notes in Mathematics*: vol. 1954, pp. 309–452, Springer-Verlag, Heidelberg, 2008.
- [18] N.B. Lovett, S. Cooper, M. Everitt, M. Trevers, and V. Kendon, “Universal quantum computation using the discrete-time quantum walk,” *Phys. Rev.*, vol. A 81, 042330, 2010.

- [19] K. Manouchehri and J.B. Wang, “Physical Implementation of Quantum Walks,” Springer-Verlag, Heidelberg, 2013.
- [20] L. Matsuoka, T. Kasajima, M. Hashimoto, and K. Yokoyama, “Numerical study on quantum walks implemented on cascade rotational transitions in a diatomic molecule,” *J. Korean Phys. Soc.*, vol. 59, pp. 2897–2900, 2011.
- [21] R. Portugal, “Quantum walks and search algorithms,” Springer-Verlag, New York, 2013.
- [22] A. Schreiber, A. Gabris, P.-P. Rohde, K. Laiho, M. Stefanak, V. Potocek, C. Hamilton, I. Jex, and C. Silberhorn, “A 2D quantum walk simulation of two-particle dynamics,” *Science*, vol. 336, 55, 2012.
- [23] N. Shenvi, J. Kempe, and K.B. Whaley, “Quantum random-walk search algorithm,” *Phys. Rev.*, vol. A 67, 052307, 2003.
- [24] S.E. Venegas-Andraca, “Quantum walks: A comprehensive review. Quant. Inform,” *Process*, vol. 11, pp. 1015–1106, 2012.