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Quantum Searching on Markov Chains — The Complete Graph

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We will give an introduction into the quantum search algorithms on the Markov chains introduced by Szegedy and recent modifications based on partially absorbing Markov chains due to Krovi et al. [Algorithmica 74, 851 \(2016\)](#) It has been shown that a quantum search can find a set of marked vertices quadratically faster (in units of the hitting time) for any reversible Markov chain. The proofs are based on certain properties of the stationary state of the partially absorbing walk and rely on quantum phase estimation techniques. We will offer an alternative view of the underlying mechanism of the quantum search based on spectral properties of the quantum walk operator. By considering the complete graph as an example, we identify the relevant two-level quantum subspace leading to a Grover-like rotation in the underlying vector space.

topics: quantum search, quantum walk, absorbing Markov chain, complete graph

1. Introduction

Grover's search finds m marked items in an unstructured data-base of N items in $\mathcal{O}(\sqrt{N})$ steps and thus quadratically faster than any classical search [1]. The algorithm was later extended to searching marked items on regular networks [2] and on random graphs above the percolation threshold [3]. The mechanism behind the search is the same in all these cases [4]: the marked vertices act as a low-rank perturbation and the system is fine-tuned such that a state localised at the marked vertices is forming an avoided crossing with an extended state uniformly covering the whole graph. The two participating eigenstates of the perturbed system become a mixture of the unperturbed states with a gap of order $\mathcal{O}(1/\sqrt{N})$. The Grover rotation can now be performed in this effectively two-dimensional sub-space if the ground state of the unperturbed system is separated from the rest of the spectrum by again at least $\mathcal{O}(1/\sqrt{N})$. The search algorithm can also be used in a transmitter-receiver configuration without any routing information guiding the signal [3, 4].

A different class of search algorithms introduced by Szegedy in 2004 [5] has received a lot of attention recently. It is based on a quantisation mechanism for ergodic and reversible Markov chains with absorbing marked vertices. Szegedy's quantum walk can detect the presence of absorbing vertices and this

leads to a solution of the detection problem, i.e., the problem of deciding, whether marked vertices are present, quadratically faster than the so-called *classical hitting time*.

Extending the notion from fully absorbing to partially absorbing vertices, Krovi et al. [6] introduced an interpolated quantum walk operator and proposed an algorithm based on the phase estimation technique [7, 8]. They achieved a quadratic speed-up — again with respect to the classical hitting time — for finding a marked vertex. However, their achievement is limited to graphs with exactly one marked vertex. Later, in a series of papers [9–11], quantum walk search algorithms based on the quantum fast-forwarding technique (QFF) [10, 12] were suggested and proven to be able to find a marked vertex in any reversible Markov chain with any number of marked vertices quadratically faster than the classical hitting time. The basic idea of the algorithms can be roughly described as follow: the QFF connects the quantum mechanical probability of finding a vertex at a time of order \sqrt{t} with the probability that the classical random walk starting from a set of unmarked vertices goes through any of the marked vertices at time t and then returns to the unmarked vertices at time $2t$. The proof is, however, quite involved and gives little intuition into the underlying mechanism. We also would like to mention a related proof based on an electric network analogy presented in [13].

We will introduce here a different approach towards understanding the mechanisms behind the quantum search for interpolated quantum Markov chains with any number of marked vertices. We analyse the walk operator in terms of its spectral decomposition. We will show results here only for a special case, the complete graph with equal transition probability between all vertices apart from self-loops. This system can be solved analytically and gives insight into the search mechanism from a spectral point of view. We think that the mechanism uncovered, revealing — like in the Grover search — a rotation in a two-dimensional invariant subspace, applies also in more general cases.

2. Quantum walk operator for a general reversible Markov chain

In this section we will introduce the quantum walk operator for an interpolated Markov chain with m marked vertices following the treatment in [6]. The walk is defined on a graph X with a set of n vertices and a set of edges E . As usual for quantum walk and quantum graph treatments, see for example [14], we introduce a vertex and edge space, \mathcal{H}_V and \mathcal{H}_E , respectively, and an associated basis, i.e., $\mathcal{H}_V = \text{span}\{|x\rangle, x \in X\}$ and $\mathcal{H}_E = \text{span}\{|xy\rangle, (xy) \in E, x, y \in X\}$. The classical Markov process is defined on \mathcal{H}_V whereas the quantum walk and the associated quantum search algorithm is defined on \mathcal{H}_E . We will first introduce the classical walk and then, following [5] and [6], construct the related unitary quantum walk operator on \mathcal{H}_E .

2.1. Absorbing Markov chain

We start with the interpolated Markov chain as introduced in [6], where a set of m vertices is marked by making these vertices partially absorbing. Starting from a general transition matrix P^0 on X , we define

$$P(s) = (1 - s)P^0 + sP', \quad 0 \leq s \leq 1, \quad (1)$$

where the elements of $P(s)$, $P_{xy}(s)$ denote the transition probability from a vertex x to a vertex y and P' is the absorbing walk as defined below. In matrix notation, we may write (1) in the block form

$$P(s) = \begin{pmatrix} P_{UU}^0 & P_{UM}^0 \\ (1 - s)P_{MU}^0 & (1 - s)P_{MM}^0 + s\mathbb{I} \end{pmatrix}, \quad (2)$$

where U and M denote the set of unmarked and marked vertices, P_{UU}^0 and P_{MM}^0 are square matrices of dimension $(n - m)$ and m , respectively. We recover the original walk at $s = 0$, whereas the marked vertices become fully absorbing at $s = 1$.

In the following we will restrict the original Markov chain P^0 to be ergodic and reversible. The latter condition implies the detailed balance relation

$$\pi_x P_{xy}^0 = \pi_y P_{yx}^0, \quad (3)$$

where π_x, π_y are the x, y components of the stationary distribution $\langle \pi |$, the left eigenvector of P^0 corresponding to the unique eigenvalue 1. It can be shown that the absorbing walk $P(s)$ also fulfills the ergodicity and reversibility condition for $0 \leq s < 1$ with associated stationary distribution $\langle \pi(s) |$, which is known analytically [6].

Next we introduce the symmetric discriminant matrix $D(s)$, i.e.,

$$D_{xy}(s) = \sqrt{P_{xy}(s)P_{yx}(s)} \quad (4)$$

with eigenvalues $\lambda_j(s)$ and associated eigenvectors $|w_j\rangle$ for $j = 1, \dots, n$. The reversibility condition (2) ensures that the matrices $P(s)$ and $D(s)$ are related by a similarity transformation. It follows that their eigenvalues $\lambda_j(s)$ coincide and in particular are real. We will use the ordering convention $1 = \lambda_n(s) \geq \lambda_{n-1}(s) \geq \dots \geq \lambda_1(s)$.

2.2. Quantum walk

We will next discuss a quantum walk associated with the classical Markov process $P(s)$. Following Szegedy [5], we define a state $|\Psi_x(s)\rangle$ in the edge space \mathcal{H}_E related to each vertex $x \in V$, i.e.,

$$|\Psi_x(s)\rangle = \sum_y \sqrt{P_{xy}(s)} |yx\rangle, \quad (5)$$

where $|xy\rangle \in \mathcal{H}_E$ denotes $|x\rangle \otimes |y\rangle$. We have

$$\langle \Psi_x(s) | \Psi_{x'}(s) \rangle = \delta_{xx'}. \quad (6)$$

To construct the unitary time evolution operator, i.e., the quantum walk operator on the edges, we first introduce the shift operator S and the coin flip operator $C(s)$ defined as

$$S|yx\rangle = |xy\rangle,$$

$$C(s) = 2 \sum_x |\Psi_x(s)\rangle \langle \Psi_x(s)| - \mathbb{I}, \quad (7)$$

where \mathbb{I} is the identity operator in \mathcal{H}_E . Operators S and $C(s)$ are both unitary [6]. The time evolution operator is then defined as

$$U(s) = SC(s). \quad (8)$$

To understand the mechanism behind the search as laid out for the complete graph in Sect. 3, it is important to gather information about the spectrum of U and its connection to the spectrum of D . It is known that the operator $U(s)$ has an invariant subspace of dimension $(2n - 1)$ [5, 6]. This subspace is spanned by the vectors $\{|v_{j\pm}(s)\rangle, |v_n(s)\rangle\}$ in \mathcal{H}_E , where

$$|v_{j\pm}(s)\rangle \equiv \frac{1}{\sqrt{2}} \left(|v_j(s)\rangle - (\pm i) |v_j^\perp(s)\rangle \right) \quad (9)$$

with $j = 1, \dots, n - 1$ and

$$|v_j(s)\rangle = \sum_x |\Psi_x(s)\rangle w_{xj}(s), \quad (10)$$

is related to the eigenvectors $|w_j(s)\rangle$ of $D(s)$, $j = 1, \dots, n$. Furthermore $|v_j^\perp(s)\rangle$ is a normalized vector perpendicular to $|v_j\rangle$, to be specified in more detail in Appendix. These vectors satisfy the orthogonality conditions

$$\begin{aligned} \langle v_{j\pm}(s)|v_{j'\pm}(s)\rangle &= \delta_{jj'}, \quad \langle v_{j\pm}(s)|v_{j'\mp}(s)\rangle = 0, \\ \langle v_n(s)|v_{j\pm}(s)\rangle &= 0, \quad \langle v_n(s)|v_n(s)\rangle = 1, \end{aligned} \quad (11)$$

see the Appendix.

The vectors $|v_{j\pm}(s)\rangle$ and $|v_n(s)\rangle$ form a part of the eigenbasis of $U(s)$, we have

$$U(s)|v_n(s)\rangle = |v_n(s)\rangle, \quad (12)$$

$$U(s)|v_{j\pm}(s)\rangle = e^{\pm i\theta_j(s)}|v_{j\pm}(s)\rangle, \quad (13)$$

where the eigenphases $\theta_j(s)$ are related to the eigenvalues of the discriminant matrix $D(s)$ by the relation

$$\lambda_j(s) = \cos(\theta_j(s)), \quad (14)$$

see Appendix for more details. We note in passing that all other eigenvalues of $U(s)$ are ± 1 .

Next we consider the time evolution of an initial state related to the stationary distribution defined as

$$|\psi(t=0)\rangle = \sum_x |\Psi_x(s)\rangle \sqrt{\pi_x}, \quad (15)$$

where $|\sqrt{\pi}\rangle$ is the eigenvector of $D(s=0)$ with $\lambda_n = 1$ and we have the natural association $\langle x|\sqrt{\pi}\rangle = \sqrt{\pi_x}$ with π_x being the x component of the stationary distribution $\langle \pi|$ of P^0 . Using (10) and the relation (4), we can expand $|\Psi_x(s)\rangle$ in terms of the eigenstates of the relevant part of the spectrum of $U(s)$, i.e.,

$$\begin{aligned} |\Psi_x(s)\rangle &= w_{xn}(s)|v_n(s)\rangle \\ &+ \sum_{j=1}^{n-1} \frac{1}{\sqrt{2}} w_{xj}(s) \left(|v_{j+}(s)\rangle + |v_{j-}(s)\rangle \right). \end{aligned} \quad (16)$$

The time evolution of $|\psi(0)\rangle$ is then given as

$$\begin{aligned} U^t(s)|\psi(0)\rangle &= a_n |v_n(s)\rangle \\ &+ \sum_{j=1}^{n-1} a_j(s) \left[\cos(\theta_j(s)t) |v_j(s)\rangle \right. \\ &\left. + \sin(\theta_j(s)t) |v_j^\perp(s)\rangle \right], \end{aligned} \quad (17)$$

where $a_j(s) = \langle w_j(s)|\sqrt{\pi}\rangle$ for $j = 1, \dots, n$.

The probability of finding the marked vertices at time t is then written as

$$P_M(t, s) = \sum_{x \in M} \sum_y \left| \langle y, x | U^t(s) | \psi(0) \rangle \right|^2. \quad (18)$$

Note that all quantities in $P_M(t, s)$ can be expressed in terms of information obtainable from the $D(s)$ matrix. Hence, it is important to understand the spectral properties of $D(s)$ in order to analyse $P_M(t, s)$ and thus the efficiency of any potential search algorithm. In the following, we will do this explicitly for the complete graph for which both the spectrum of $D(s)$ and the mechanisms behind a quantum search can be worked out analytically.

3. Uniform Markov chains on a complete graph with m marked vertices

3.1. The setup and the spectrum of $D(s)$

We will now consider the special case of a quantum search on a complete graph where every vertex is connected to every other vertex. We focus here on an unperturbed Markov process P^0 with n vertices, where we chose the transition probabilities between vertices to be uniform. The corresponding transition matrix has the form

$$\begin{aligned} P^0 &= pI + \frac{1-p}{n-1}(J-I) = \\ &\frac{np-1}{n-1}I + \frac{1-p}{n-1}J, \end{aligned} \quad (19)$$

where J is the all-ones matrix, I is the identity matrix, and p is a real number such that $0 \leq p \leq 1$. Note that the complete graph without self-loops corresponds to the special case $p = 0$.

Let us assume that there are m marked vertices. The eigenvalues and eigenvectors of the discriminant matrix $D(s)$ of the interpolated Markov chain $P(s)$ derived from (19) as defined in (1) can be given explicitly. After some calculation, we obtain the following eigenvalues and eigenvectors,

index j	eigenvalue λ_j	eigenvector $ w_j\rangle$
$1, \dots, n-m-1$	$\frac{np-1}{n-1}$	$ \mathbf{z}_{n-m}, \mathbf{0}_m\rangle$
$n-m$	$\frac{np-1}{n-1} + \frac{1-p}{n-1}(n-m)s$	$\alpha \left -\sqrt{\frac{m}{n-m}} \mathbf{1}_{n-m}, \sqrt{\frac{n-m}{m}} \sqrt{1-s} \mathbf{1}_m \right\rangle$
$n-m+1, \dots, n-1$	$(1-s)\frac{np-1}{n-1} + s$	$ \mathbf{0}_{n-m}, \mathbf{z}_m\rangle$
n	1	$\alpha \left \sqrt{1-s} \mathbf{1}_{n-m}, \mathbf{1}_m \right\rangle$

Here, $\mathbf{1}_k$ and $\mathbf{0}_k$ denote a k -dimensional vector with entries being either all one or all zero, respectively. Furthermore, \mathbf{z}_k denotes a $k-1$ dimensional set of normalized k -dimensional vectors with $\sum_{i=1}^k z_i = 0$.

The normalization constant α is given as

$$\alpha = \frac{1}{\sqrt{n}} \frac{1}{\sqrt{1-s(1-p_M)}}. \quad (21)$$

Here $p_M = m/n$, which is the probability to pick a marked element from the stationary distribution [6]. We will see in the next section that only two states facilitate the actual search, i.e., the states $|w_n\rangle$ and $|w_{n-m}\rangle$, respectively. We find in particular that the stationary distribution at $s = 0$ is uniformly distributed, i.e.,

$$|\sqrt{\pi}\rangle = \frac{1}{\sqrt{n}}|\mathbf{1}_n\rangle. \quad (22)$$

3.2. Quantum search as a rotation in a 2D subspace of quantum walk operator

We will now address the mechanism behind a quantum search in the absorbing vertex formalism for this particular example. We will show that — like for Grover's search — the search can be understood as a rotation in an effectively two-dimensional invariant subspace of the quantum walk operator at a specific interpolation parameter s_0 . This is akin to the avoided crossing approach discussed in [4, 15], however, we will show below, that here the mechanism is not facilitated by an avoided crossing. Indeed, just considering the spectrum (20), it is easy to see that there are no avoided crossings present as all eigenvalues vary linearly with the parameter s .

We start by defining the initial and target state, respectively,

$$|v_{\text{ini}}\rangle = \sum_x |\Psi_x\rangle \sqrt{\pi_x} = \frac{1}{\sqrt{n}} \sum_x |\Psi_x\rangle, \quad (23)$$

and

$$|v_{\text{fin}}\rangle = \frac{1}{\sqrt{m}} \sum_{x \in M} |\Psi_x\rangle. \quad (24)$$

We find immediately using (20) that

$$\langle v_j | v_{\text{ini}} \rangle = \langle v_j | v_{\text{fin}} \rangle = 0 \quad \text{for all } j \neq n, n-m. \quad (25)$$

Both the initial and the target state are in the subspace spanned by $|v_n\rangle$ and $|v_{n-m}\rangle$. Note that $|v_{n-m}\rangle$ is not an eigenvector of U , only the individual states $|v_{(n-m)\pm}\rangle$ are.

In order to find the optimal s parameter as well as the search time t , we write $|v_n(s)\rangle$ and $|v_{n-m}(s)\rangle$ in terms of the initial and final states. Thus,

$$|v_n(s)\rangle = c_1 |v_{\text{ini}}(s)\rangle + c_2 |v_{\text{fin}}(s)\rangle, \quad (26)$$

$$|v_{n-m}(s)\rangle = c_3 |v_{\text{ini}}(s)\rangle + c_4 |v_{\text{fin}}(s)\rangle. \quad (27)$$

where the c_i 's are obtained as

$$c_1 = \frac{1}{\sqrt{1-p_M}} \sin(\phi),$$

$$c_2 = \frac{1}{\sqrt{1-p_M}} \left[\sqrt{1-p_M} \cos(\phi) - \sqrt{p_M} \sin(\phi) \right],$$

$$c_3 = \frac{1}{\sqrt{1-p_M}} \cos(\phi),$$

$$c_4 = \frac{-1}{\sqrt{1-p_M}} \left[\sqrt{1-p_M} \sin(\phi) + \sqrt{p_M} \cos(\phi) \right], \quad (28)$$

where

$$\begin{aligned} \cos(\phi) &= \frac{\sqrt{p_M}}{\sqrt{1-s(1-p_M)}}, \\ \sin(\phi) &= \frac{\sqrt{(1-s)(1-p_M)}}{\sqrt{1-s(1-p_M)}}. \end{aligned} \quad (29)$$

The optimal s parameter is obtained by demanding that the two vectors $|v_n(s)\rangle$ and $|v_{n-m}(s)\rangle$ are maximally mixed with the initial and final states up to a change in sign, i.e.,

$$c_1 = c_2 \quad \text{and} \quad c_3 = -c_4. \quad (30)$$

A straightforward calculation shows that both conditions are in fact equivalent, i.e., we obtain the optimal s_0 by solving

$$\sin(\phi) = \sqrt{1-p_M} \cos(\phi) - \sqrt{p_M} \sin(\phi), \quad (31)$$

which leads to

$$s_0 = 1 - \left(\frac{\sqrt{p_M}}{1 + \sqrt{p_M}} \right)^2. \quad (32)$$

At the optimal s_0 with associated angle $\phi_0 = \phi(s_0)$, we thus obtain

$$|v_{\text{ini}}\rangle = \cos(\phi_0) |v_n(s_0)\rangle + \sin(\phi_0) |v_{n-m}(s_0)\rangle, \quad (33)$$

$$|v_{\text{fin}}\rangle = \cos(\phi_0) |v_n(s_0)\rangle - \sin(\phi_0) |v_{n-m}(s_0)\rangle. \quad (34)$$

Note that the coefficients of $|v_{\text{ini}}\rangle$ and $|v_{\text{fin}}\rangle$ at $s = s_0$ agree up to a sign change.

Since the vectors $|v_j(s)\rangle$ are related to the eigenvectors of $D(s)$, $|w_j(s)\rangle$, by (10), the invariant subspace can be represented in the plane spanned by the two vectors $|w_n(0)\rangle$ and $|w_{n-m}(0)\rangle$. The initial and final states in the reduced vertex space can be written as

$$|v_{\text{ini}}\rangle = |w_n(0)\rangle, \quad |v_{\text{fin}}\rangle = |w_n(1)\rangle, \quad (35)$$

The states (35) can be represented by $|w_n(0)\rangle$, $|w_n(1)\rangle$, and $|w_n(s)\rangle$ as in Fig. 1. The angles between $|w_n(1)\rangle$, $|w_n(s)\rangle$ and $|w_n(0)\rangle$, $|w_n(s)\rangle$ stay the same when changing s and are equal at the optimal $s = s_0$. The angle δ in Fig. 1 is then given as $\tan \delta = \sqrt{\frac{p_M}{1-p_M}}$.

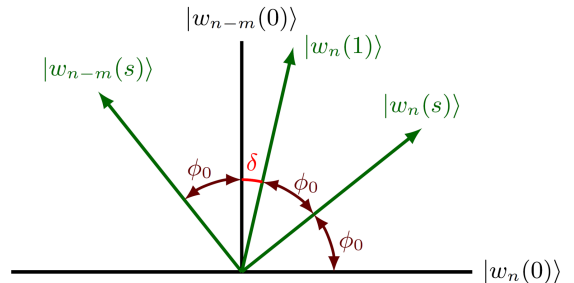


Fig. 1. Geometrical interpretation of the maximal mixing. The angles between $|w_n(1)\rangle$ and $|w_n(s)\rangle$ and $|w_n(0)\rangle$ and $|w_n(s)\rangle$ coincide at the optimal $s = s_0$. The angle δ is given as $\tan \delta = \sqrt{\frac{p_M}{1-p_M}}$.

Next, let us determine the searching time t_s from the initial state $|v_{\text{ini}}(s)\rangle$ to the final state $|v_{\text{fin}}(s)\rangle$ at the optimal s_0 . The time evolution of the initial state $|v_{\text{ini}}\rangle$ can be written as

$$U^t |v_{\text{ini}}(s_0)\rangle = a_c |v_n(s_0)\rangle + a_s \left(\cos(\theta_{n-m}t) |v_{n-m}(s_0)\rangle + \sin(\theta_{n-m}t) |v_{n-m}^\perp(s_0)\rangle \right), \quad (36)$$

where $a_c = \cos(\phi)(s_0)$ and $a_s = \sin(\phi)(s_0)$ and $\theta_{n-m} = \theta_{n-m}(s_0)$. By requiring $\cos(\theta_{n-m}t) = -1$, equivalently $\sin(\theta_{n-m}t) = 0$, at the search time

$$t_s = \frac{\pi}{\theta_{n-m}(s_0)}, \quad (37)$$

we obtain

$$U^{t_s}(s_0) |v_{\text{ini}}\rangle = a_c |v_n(s_0)\rangle - a_s |v_{n-m}(s_0)\rangle = |v_{\text{fin}}\rangle. \quad (38)$$

For large n , when taking $\theta_{n-m}(s_0) \approx \sqrt{2(1 - \lambda_{n-m}(s_0))}$ and

$$\lambda_{n-m}(s) \approx 1 - \frac{2n}{n-1}(1-p)p_M, \quad (39)$$

we find that the search time t_s can be approximately written as

$$t_s \approx \frac{\pi}{2} \sqrt{\frac{1}{(1-p)}} \sqrt{\frac{n}{m}}. \quad (40)$$

The search time for a quantum search on a complete graph is thus proportional to \sqrt{n} . At the optimal value s_0 , the probability to find at least one marked vertices is given by

$$P_M(t_s, s_0) = \sum_{x \in M} \sum_y |\langle y, x | v_{\text{fin}} \rangle|^2 = 1. \quad (41)$$

Thus, at $t = t_s$ and $s = s_0$, we find all marked vertices of the complete graph simultaneously.

Note that, for large n , the classical hitting time is proportional to n , i.e.,

$$HT(P, M) = \frac{n-1}{(1-p)m} \stackrel{n \rightarrow \infty}{\approx} \frac{1}{(1-p)} \frac{n}{m}. \quad (42)$$

This shows that a quantum search is quadratically faster than a classical search as expected.

4. Conclusions

The spectral analysis presented here for the complete graph leads to a comprehensive understanding of the quantum walk operator: the operator acts as a rotation in each of the $n-1$ two-dimensional invariant subspaces spanned by pairs of eigenstates. The time-evolution of the initial state can be expressed in terms of the eigenstates of the discriminant matrix, which implies that the search algorithm can be understood in terms of these invariant subspaces alone.

We investigate the influence of these eigenspaces on the quantum search mechanism in detail for the complete graph problem; here, we show, that only two eigenspaces are relevant for the quantum search

starting from the initial stationary distribution. The interpolation parameter s can be interpreted as a rotation angle of the two relevant eigenvectors in the two-dimensional space spanned by the vectors corresponding to the initial and the final states. The optimal value of s can be determined from the condition of maximal mixing of the initial and final vectors with the two relevant eigenvectors. The optimal search time is then proportional to the inverse of the gap between the eigenphases of these eigenvectors. It is of the order $\sqrt{n/m}$ in the quantum case while the classical hitting time is of the order n/m .

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Appendix: Construction of the invariant subspace of $U(s)$

In this appendix, some relations to be used in deriving the eigen-system of the walk operator $U(s)$ are found. We will omit the parameter s for simplicity.

We will give more details regarding the eigenvectors and eigenvalues of the operator U and their connection to the spectrum of D . To do so, we start with some relations also given in [6]. Using that $|\Psi_x\rangle = \sum_x \sqrt{P_{xy}} |y, x\rangle$ and $\sum_y P_{xy} = 1$, one can show that

$$\langle \Psi_x | \Psi_y \rangle = \delta_{xy}, \quad (43)$$

$$\langle \Psi_x | S | \Psi_y \rangle = D_{xy}. \quad (44)$$

Using (44) together with $S^2 = 1$, and by expressing $|v_j\rangle$ as $|v_j\rangle = \sum_x |\Psi_x\rangle w_{xj}$, one can show that

$$\langle v_i | S | v_j \rangle = \lambda_j \delta_{ij}, \quad (45)$$

where λ_j is the corresponding eigenvalue of D . By using $C = 2 \sum_x |\Psi_x\rangle \langle \Psi_x| - I$ and (44), we obtain

$$C |v_j\rangle = |v_j\rangle, \quad (46)$$

$$CS |v_j\rangle = 2\lambda_j |v_j\rangle - S |v_j\rangle. \quad (47)$$

Now, let us construct the normalized vector $|v_j^\perp\rangle$ perpendicular to $|v_j\rangle$. Due to (45), the vector $S |v_j\rangle$ has a component of size λ_j in the $|v_j\rangle$ direction, so we can write formally

$$S |v_j\rangle = \lambda_j |v_j\rangle + b_j |v_j^\perp\rangle. \quad (48)$$

From $\langle v_i | S^2 | v_j \rangle = \delta_{ij}$, we obtain

$$b_j = \sqrt{1 - \lambda_j^2}. \quad (49)$$

Therefore, the vector $|v_j^\perp\rangle$ is given by

$$|v_j^\perp\rangle = \frac{1}{\sqrt{1 - \lambda_j^2}} \left(\lambda_j |v_j\rangle - S |v_j\rangle \right), \quad (50)$$

for $j < n$. In the case $j = n$, $|v_n\rangle$ itself is an eigenvector of U . Note that $\lambda_n = 1$. The actions of the operators C and S on $|v_j\rangle$ and $|v_j^\perp\rangle$ are given by

$$S|v_j^\perp\rangle = \sqrt{1 - \lambda_j^2}|v_j\rangle - \lambda_j|v_j^\perp\rangle \quad (51)$$

$$C|\tilde{v}_j\rangle = -|v_j^\perp\rangle \quad (52)$$

for $j < n$.

Next, let us construct the eigenspace of $U = SC$ using a geometrical point of view. From (46) and (47), we see that

$$U|v_j\rangle = S|v_j\rangle, \quad (53)$$

$$US|v_j\rangle = 2\lambda_j S|v_j\rangle - |v_j\rangle, \quad (54)$$

which implies that the subspace spanned by $\{|v_j\rangle, S|v_j\rangle\}$ is invariant under $U = SC$. For a given j the invariant subspace is a two-dimensional plane, so there is a vector perpendicular to $|v_j\rangle$, which is the vector $|v_j^\perp\rangle$ as derived above.

Now, let us consider the action of C and S on a vector $|\tilde{v}_j\rangle$ written as $|\tilde{v}_j\rangle = a|v_j\rangle + b|v_j^\perp\rangle$ in this plane, where a and b are constants. Using (46) and (51), we can see that the action of C on $|\tilde{v}_j\rangle$ is given by

$$C|\tilde{v}_j\rangle = a|v_j\rangle - b|v_j^\perp\rangle, \quad (55)$$

which is just the reflection about the $|v_j\rangle$ axis as in Fig. 2. In matrix notation, the action of C can be written as

$$R_C = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (56)$$

The action of S on $|\tilde{v}_j\rangle$, using (48) and (51), is given by

$$\begin{aligned} S|\tilde{v}_j\rangle &= a(\cos(\theta_j)|v_j\rangle + \sin(\theta_j)|v_j^\perp\rangle) \\ &+ b(\sin(\theta_j)|v_j\rangle - \cos(\theta_j)|v_j^\perp\rangle) = \\ &(\cos(\theta_j)a + \sin(\theta_j)b)|v_j\rangle \\ &+ (\sin(\theta_j)a - \cos(\theta_j)b)|v_j^\perp\rangle \end{aligned} \quad (57)$$

with $\lambda_j = \cos(\theta_j)$. Note that the eigenvalues λ_j are real with $|\lambda_j| \leq 1$ by virtue of the transition matrix P representing a reversible Markov chain.

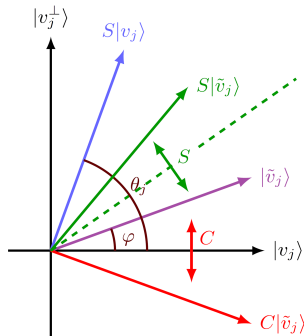


Fig. 2. Geometrical interpretation of the action of C and S in the plane spanned by $|v_j\rangle$ and $|v_j^\perp\rangle$. The action of C is the reflection about the $|v_j\rangle$ axis. The action of S is the reflection about a line (dashed line in green) through the origin, where the line makes an angle $\theta_j/2$ with the $|v_j\rangle$ axis. Note that the angle of $S|v_j\rangle$ with respect to $|v_j\rangle$ is θ_j .

In matrix notation, the action of S can be written as

$$\begin{aligned} \begin{bmatrix} a' \\ b' \end{bmatrix} &= \begin{bmatrix} \cos(\theta_j) & \sin(\theta_j) \\ \sin(\theta_j) & -\cos(\theta_j) \end{bmatrix} = \\ \begin{bmatrix} a \\ b \end{bmatrix} &\equiv R_S(\theta_j) \begin{bmatrix} a \\ b \end{bmatrix} \end{aligned} \quad (58)$$

representing a reflection about the line through the origin making an angle $\theta_j/2$ with the $|v_j\rangle$ axis as shown in Fig. 2.

Therefore, the action of the SC on a vector in the plane spanned by $|v_j\rangle$ and $|v_j^\perp\rangle$ represents a product of two reflection matrices, that is,

$$\begin{aligned} SC \rightarrow R_S(\theta_j)R_C &= \\ \begin{bmatrix} \cos(\theta_j) & \sin(\theta_j) \\ \sin(\theta_j) & -\cos(\theta_j) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} &= \\ \begin{bmatrix} \cos(\theta_j) & -\sin(\theta_j) \\ \sin(\theta_j) & \cos(\theta_j) \end{bmatrix} &\equiv R(\theta_j) \end{aligned} \quad (59)$$

which is just the rotation about the origin by an angle θ_j . Hence, the action of the quantum walk operator $U = SC$ on a vector in the plane $|v_j\rangle - |v_j^\perp\rangle$ can be represented as a rotation composed of two reflection operations $R_S(\theta_j)$ and R_C . It is the same action as in Grover's algorithm [1] (see Fig. 2).

The eigenvectors and eigenvalues in each of the j sub-spaces can now be obtained from the eigenvectors and eigenvalues of the rotation matrix $R(\theta_j)$, i.e.,

$$\begin{aligned} \text{Eigenvector: } \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm i \end{bmatrix} & \quad \text{Eigenvalue: } e^{\mp i\theta_j}, \\ & \quad (60) \end{aligned}$$

In terms of the $|v_j\rangle, |v_j^\perp\rangle$ basis, the eigenvectors of U then have the form

$$|v_{j\pm}\rangle = \frac{1}{\sqrt{2}}(|v_j\rangle - (\pm i)|v_j^\perp\rangle) \quad (61)$$

with corresponding eigenvalues $e^{\pm i\theta_j}$. For $j = n$, we can easily show that $|v_n\rangle$ itself is the eigenvector with eigenvalue 1. There are two eigenstates corresponding to the index $j < n$, but for $j = n$, there is only one state. Therefore, the dimension of the invariant subspace of U is $2n - 1$.

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