

Multimarked Spatial Search by Continuous-Time Quantum Walk

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Abstract

The quantum-walk-based spatial search problem aims to find a marked vertex using a quantum walk on a graph with marked vertices. We describe a framework for determining the computational complexity of spatial search by continuous-time quantum walk on arbitrary graphs by providing a recipe for finding the optimal running time and the success probability of the algorithm. The quantum walk is driven by a Hamiltonian that is obtained from the adjacency matrix of the graph modified by the presence of the marked vertices. The success of our framework depends on the knowledge of the eigenvalues and eigenvectors of the adjacency matrix. The spectrum of the modified Hamiltonian is then obtained from the roots of the determinant of a real symmetric matrix, whose dimension depends on the number of marked vertices. We show all steps of the framework by solving the spatial searching problem on the Johnson graphs with fixed diameter and with two marked vertices. Our calculations show that the optimal running time is $O(\sqrt{N})$ with asymptotic probability $1 + o(1)$, where N is the number of vertices.

Keywords: Continuous-time quantum walk, spatial quantum search, Johnson graph, multiple marked vertices

1 Introduction

Farhi and Gutmann [1] introduced the continuous-time quantum walk as a discrete-space version of the Schrödinger equation, where the positions of the particle are the vertices of a graph, more specifically, a tree whose nodes represent solutions to a decision problem [2]. Childs and Goldstone [3] used the continuous-time quantum walk to address the spatial search problem with one marked vertex, the goal of which is to find the marked vertex when the walk departs from an initial state that is easy to prepare. The evolution is based on a modified Hamiltonian, which has an extra term that depends on the location of the marked vertex and is different from the one used by Farhi and Gutmann, which is based only on the graph's adjacency matrix. Childs and Goldstone analyzed the search on lattices, hypercubes, and the complete graph to determine

whether the quantum-walk-based search algorithm is quicker than the random-walk-based one on the same graphs, obtaining negative results in some cases, for instance, on d -dimensional lattices with $d \leq 4$. This cannot be taken as proof that it is impossible to find a quantum-walk-based search algorithm that provides a speedup over the best random-walk-based case. Indeed, using alternative discrete-time quantum walk models it is possible to achieve a quadratic speedup for d -dimensional lattices with $d \geq 2$ [4, 5].

The origin of the quantum-walk-based spatial search problem is a combination of Farhi and Gutmann's proposal in 1998 of speeding up random walks on decision trees by using a continuous-time quantum walk [1] together with Benioff's proposal in 2000 of applying Grover's algorithm [6] with the goal of speeding up classical search algorithms for a marked vertex on the two-dimensional lattice [7]. After the contribution of those authors, the area of quantum-walk-based spatial search algorithms has split into two different formulations in the literature, both of which are important because they reveal different computational and mathematical aspects of quantum walks.

The first formulation asks whether the number of steps that a quantum walk on a graph G takes to find a marked vertex is less than the number of steps that a classical random walk takes on the same graph G . This formulation was introduced by Shenvi et al. [8], who showed that a quantum walk on a hypercube finds a marked vertex quicker than a random walk. In a context close to the spatial search algorithm, Childs et al. [9] showed that the propagation of a particle between a particular pair of nodes is exponentially faster when driven by a continuous-time quantum walk compared to a random walk. There are many papers in the literature addressing this formulation in both the discrete-time [8, 10, 11, 12] and continuous-time [3, 13, 14, 15, 16, 17, 18, 19, 20, 21] cases. Experimental implementations of search algorithms by continuous-time quantum walk are described in [22, 23, 24, 25].

The second formulation asks whether the number of steps that a classical random walk on a graph G takes to find a marked vertex $v \in V(G)$ can be improved by using a quantum walk on any graph G' , so that the quantum walk on G' would uncover the necessary information to find the vertex v in the original graph G . This formulation was introduced by Szegedy [26], who showed that the quantum hitting time of a quantum walk on the bipartite graph G' obtained from a graph G , where the random walk takes place, is quadratically less than the classical hitting time. To find a marked vertex, it is still necessary to show that the success probability is $\Omega(1)$. Many papers in the literature have addressed the second formulation in both the discrete-time [27, 28, 29, 30] and continuous-time [31, 32] cases, and in all of those papers the quantum walk takes place on a bipartite graph G' obtained from G via a duplication process and the random walk takes place on an almost arbitrary graph G with multiple marked vertices. Ambainis et al. [30] provided a closure of Szegedy's problem by showing that there is a quadratic speedup for finding a marked vertex with success probability $\tilde{\Omega}(1)$ on an arbitrary graph G by discrete-time quantum walk on G' . Apers et al. [32] go along the same line by continuous-time quantum walk.

In this work, we address the first formulation of the spatial search problem by continuous-time quantum walk on arbitrary graphs with multiple marked vertices and we outline a framework to determine the computational complexity of the search algorithm that is successful if the evolution operator satisfies some asymptotic conditions. As an example of our framework, we analyze in full detail the search algorithm on the Johnson graph with two marked vertices. The framework is based on a real symmetric matrix M , which depends on the entries of the adjacency matrix and on the locations of the marked vertices. The fact that the determinant of this matrix

is zero allows us to find the spectrum of the modified Hamiltonian if we know the spectrum of the adjacency matrix. Then, we are able to find the spectral gap and all quantities necessary to determine the algorithm's optimal running time and the success probability assuming that the spectral gap tends to zero when the number of vertices increases. The relevant quantities are basically the overlaps between the marked vertices with the eigenvectors of the modified Hamiltonian.

The Johnson graph $J(n, k)$ plays an important role in quantum walks because it is used in the element distinctness algorithm [27] and in many spatial search algorithms [33, 34]. The vertices of $J(n, k)$ are k -subsets of a set with n elements and two vertices are adjacent if and only if the intersection of these vertices is a $(k - 1)$ -subset. In this work, we use the Johnson graph $J(n, k)$ with two marked vertices as an example of all steps of our framework for determining the time complexity of the spatial search algorithm by continuous-time quantum walk. We show that the optimal running time to find a marked vertex is $\pi k \sqrt{N} / 2\sqrt{2}$ with asymptotic probability $1 + o(1)$ when k is fixed.

The structure of this paper is as follows. In Sec. 2, we outline a framework for determining the computational complexity of the spatial search algorithm by continuous-time quantum walk on graphs with multiple marked vertices. In Sec. 3, we apply our framework to analyze with mathematical rigor the spatial search algorithm on the Johnson graph with two marked vertices. In Sec. 4, we present our final remarks.

2 Multimarked framework

Let $G(V, E)$ be a finite graph with vertex set V and edge set E . We associate G with a Hilbert space \mathcal{H} with computational basis $\{|v\rangle : v \in V\}$, as is usually done in the definition of the continuous-time quantum walk [1]. Let W be the set of marked vertices. We consider the time-independent Hamiltonian of the form [3]

$$H = -\gamma A - \sum_{w \in W} |w\rangle\langle w|, \quad (1)$$

where A denotes the adjacency matrix of G , and γ is a real and positive parameter. The spatial search algorithm starts with the initial state $|\psi(0)\rangle$, which is the uniform superposition of the computational basis

$$|\psi(0)\rangle = \frac{1}{\sqrt{N}} \sum_{v \in V} |v\rangle,$$

where N is the number of vertices of G . The quantum state at time t is therefore given by

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle.$$

The probability of finding a marked vertex at time t is

$$p(t) = \sum_{w \in W} |\langle w | \psi(t) \rangle|^2. \quad (2)$$

The goal of the algorithm is to find the optimal values of parameters t and γ so that the success probability is as high as possible.

2.1 Spectrum of the Hamiltonian

For an operator U , we let $\sigma(U)$ denote the spectrum of U . Suppose that the adjacency matrix A of $G(V, E)$ has exactly $k + 1$ distinct eigenvalues $\phi_0 > \phi_1 > \cdots > \phi_k$. For $0 \leq \ell \leq k$, let P_ℓ denote the orthogonal projector onto the eigenspace of A in \mathcal{H} for the eigenvalue ϕ_ℓ , that is,

$$A = \sum_{\ell=0}^k \phi_\ell P_\ell.$$

Let λ and $|\lambda\rangle$ be an eigenvalue and a normalized eigenvector of H , respectively, that is

$$H|\lambda\rangle = \lambda|\lambda\rangle$$

and $\langle \lambda | \lambda \rangle = 1$. Hamiltonian H and operator $-\gamma A$ may share common eigenvalues and eigenvectors, as shown in the next Proposition.

Proposition 1. $\lambda \in \sigma(-\gamma A)$ and $(-\gamma A)|\lambda\rangle = \lambda|\lambda\rangle$ if and only if $\langle w | \lambda \rangle = 0$ for all $w \in W$.

Proof. Using the definition of H , we obtain

$$\sum_{w \in W} |w\rangle \langle w | \lambda \rangle = -(\gamma A + H)|\lambda\rangle.$$

If $\lambda \in \sigma(-\gamma A)$ and $(-\gamma A)|\lambda\rangle = \lambda|\lambda\rangle$, the right-hand side is zero and the entries of the vector $\sum_{w \in W} |w\rangle \langle w | \lambda \rangle$ must be zero. Then, we have $\langle w | \lambda \rangle = 0$ for all $w \in W$. On the other hand, if $\langle w | \lambda \rangle = 0$ for all $w \in W$, the left-hand side is zero. Since $H|\lambda\rangle = \lambda|\lambda\rangle$, we have $\lambda \in \sigma(-\gamma A)$ and $(-\gamma A)|\lambda\rangle = \lambda|\lambda\rangle$. \square

From Eq. (2), we see that the eigenvectors $|\lambda\rangle$ such that $\langle w | \lambda \rangle = 0$ for all $w \in W$ play no role in the calculation of the probability $p(t)$ of finding a marked vertex. The eigenvalues λ associated with those eigenvectors are in the spectrum of $-\gamma A$. In the continuation, we assume that $\langle w | \lambda \rangle \neq 0$ for at least one marked vertex w . Then, $\lambda \notin \sigma(-\gamma A)$.

Using the definition of H , we obtain

$$P_\ell H|\lambda\rangle = -P_\ell \left(\gamma A + \sum_{w \in W} |w\rangle \langle w | \right) |\lambda\rangle, \quad (3)$$

and since we are assuming that $\lambda \notin \sigma(-\gamma A)$, we write the previous equation as

$$P_\ell |\lambda\rangle = -\frac{1}{\lambda + \gamma \phi_\ell} \sum_{w \in W} \langle w | \lambda \rangle P_\ell |w\rangle. \quad (4)$$

The method that we describe for calculating an eigenvalue λ of H works only if $\lambda \notin \sigma(-\gamma A)$.

Since $\sum_{\ell=0}^k P_\ell = I$, we have for a fixed marked vertex w

$$\langle w | \lambda \rangle = \sum_{\ell=0}^k \langle w | P_\ell | \lambda \rangle.$$

Then, using Eq. (4), we obtain

$$\langle w|\lambda\rangle = -\sum_{\ell=0}^k \frac{1}{\lambda + \gamma\phi_\ell} \left(\sum_{w' \in W} \langle w'|\lambda\rangle \langle w|P_\ell|w'\rangle \right),$$

which can be cast into the form

$$\sum_{w' \in W} M_{ww'}^\lambda \langle w'|\lambda\rangle = 0, \quad (5)$$

where

$$M_{ww'}^\lambda = \delta_{ww'} + \sum_{\ell=0}^k \frac{\langle w|P_\ell|w'\rangle}{\lambda + \gamma\phi_\ell}.$$

Since $\langle w|\lambda\rangle|_{w \in W}$ is a 0-eigenvector of the real symmetric matrix $M^\lambda = (M_{ww'}^\lambda)_{w, w' \in W}$, we have

$$\det(M^\lambda) = 0,$$

which can be used to determine λ .

We have shown the following proposition:

Proposition 2. *Let λ be an eigenvalue of H associated with eigenvector $|\lambda\rangle$ such that $\lambda \notin \sigma(-\gamma A)$ and $\langle w|\lambda\rangle \neq 0$ for at least one $w \in W$. Define the real symmetric matrix $M^\lambda = (M_{ww'}^\lambda)_{w, w' \in W}$, where*

$$M_{ww'}^\lambda = \delta_{ww'} + \sum_{\ell=0}^k \frac{\langle w|P_\ell|w'\rangle}{\lambda + \gamma\phi_\ell}. \quad (6)$$

Then, $\det(M^\lambda) = 0$ and $\langle w|\lambda\rangle|_{w \in W}$ is a nontrivial 0-eigenvector of M^λ .

To establish a method to find the eigenvalues of H , it is more important to us the inverse of Proposition 2. Given a graph $G(V, E)$ with a set W of marked vertices, we obtain the Hamiltonian (1) and matrix $M^{\lambda'}$ for an unknown real number λ' . Numerical calculations with random graph instances show that all roots λ' of the equation $\det(M^{\lambda'}) = 0$ such that $\lambda' \notin \sigma(-\gamma A)$ are eigenvalues of H . Indeed, the numerator of $\det(M^{\lambda'})$ is a polynomial $P(\lambda')$ of the indeterminate λ' , whose degree is $k|W|$. There are at most $k|W|$ roots of $P(\lambda') = 0$ and some of them may be in $\sigma(-\gamma A)$. Numerical calculations show that the remaining ones are in $\sigma(H)$.

2.2 Asymptotic analysis

It is natural to expect that the spectral gap of the modified Hamiltonian tends to zero when the number of vertices N increases. In this case, the analysis of the search algorithm is simpler in the asymptotic regime. Besides, in the continuation we assume that the asymptotic computational complexity of the search algorithm depends only on two eigenvalues λ^\pm closest of $-\gamma\phi_0$ so that

$$\lambda^\pm = -\gamma\phi_0 \pm \epsilon + o(\epsilon). \quad (7)$$

In this case, the spectral gap is asymptotically $2\epsilon > 0$. Matrix M^λ simplifies to

$$M_{ww'}^{\lambda^\pm} = \delta_{ww'} + \sum_{\ell=0}^k \frac{\langle w|P_\ell|w'\rangle}{\gamma(\phi_\ell - \phi_0) \pm \epsilon}.$$

Up to second order in ϵ we obtain

$$M_{ww'}^{\lambda^\pm} = \pm \frac{\langle w|P_0|w' \rangle}{\epsilon} + \delta_{ww'} - \frac{S_{ww'}^{(1)}}{\gamma} \mp \frac{\epsilon S_{ww'}^{(2)}}{\gamma^2},$$

where

$$S_{ww'}^{(1)} = \sum_{\ell=1}^k \frac{\langle w|P_\ell|w' \rangle}{\phi_0 - \phi_\ell}$$

and

$$S_{ww'}^{(2)} = \sum_{\ell=1}^k \frac{\langle w|P_\ell|w' \rangle}{(\phi_0 - \phi_\ell)^2}.$$

The goal is to find ϵ . Using $\det(M^\lambda) = 0$ and considering the numerator of up to order ϵ^2 , we obtain a quadratic equation $\epsilon^2 + a(\gamma)\epsilon - b(\gamma) = O(\epsilon^3)$, which cannot have the linear term because that is the only way to have the $\pm\epsilon$ term in Eq. (7). Then, we use the equation $a(\gamma) = 0$ to determine the optimal value of γ and then ϵ is given by $\sqrt{b(\gamma)}$.

2.3 Calculation of the computational complexity

Using an orthonormal set $\{|\lambda\rangle\}$ of eigenvectors of H , the probability of finding a marked vertex as a function of t (see Eq. (2)) is given by

$$p(t) = \sum_{w \in W} \left| \sum_{\lambda} e^{-i\lambda t} \langle w|\lambda\rangle \langle \lambda|\psi(0)\rangle \right|^2.$$

The exact eigenvalues λ are the roots of $\det(M^\lambda) = 0$, but usually the calculation of those roots is too complicated. In the continuation, we analyze the computational complexity of quantum walks on graphs that satisfy very restrictive conditions. Let us assume again that the spectral gap tends to zero when the number of vertices increases and the asymptotic success probability depends only on λ^\pm and their associated eigenvectors $|\lambda^\pm\rangle$. Besides, let us assume that asymptotically

$$\langle \lambda^+|\psi(0)\rangle \langle w|\lambda^+ \rangle = -\langle \lambda^-|\psi(0)\rangle \langle w|\lambda^- \rangle + o(1) \quad (8)$$

for all $w \in W$, which is true for the quantum walk on the Johnson graph with two marked vertices, as we show in the next Section. Under those assumptions, the probability of finding a marked vertex reduces to

$$p(t) = 4 |\langle \lambda^+|\psi(0)\rangle|^2 \sum_{w \in W} |\langle w|\lambda^+ \rangle|^2 \sin^2 \epsilon t + o(1) + o(\epsilon t). \quad (9)$$

Then, the optimal running time is

$$t_{\text{run}} = \frac{\pi}{2\epsilon} \quad (10)$$

and the success probability is

$$p_{\text{succ}} = 4 |\langle \lambda^+|\psi(0)\rangle|^2 \sum_{w \in W} |\langle w|\lambda^+ \rangle|^2 + o(1). \quad (11)$$

Although we have imposed many restrictions in order to obtain Eq. (9), there are many examples with one marked vertex [3, 34] and multimarked vertices [35] that obey all those restrictions.

Now let us focus on the calculation of $|\langle w|\lambda^+\rangle|$ and $|\langle \lambda^+|\psi(0)\rangle|$. Recall that $\langle w|\lambda^+\rangle|_{w \in W}$ is a 0-eigenvector of M^{λ^+} with entries $\langle w|\lambda^+\rangle$ for $w \in W$. Since M^{λ^+} is known, we are able to find a normalized 0-eigenvector of M^{λ^+} , which we call $|u\rangle$. Our numerical calculations support the conjecture that eigenvalue 0 has multiplicity one. Then vectors $\langle w|\lambda^+\rangle|_{w \in W}$ and $|u\rangle$ satisfy

$$\langle w|\lambda^+\rangle|_{w \in W} = c^+|u\rangle,$$

where c^+ is a complex number. Using

$$\sum_{\ell=0}^k \|P_\ell|\lambda^+\rangle\|^2 = 1,$$

$\langle w|\lambda^+\rangle = c^+ u(w)$ ($u(w)$ is the entry of $|u\rangle$ associated with w), and Eq. (4), we obtain

$$\frac{1}{|c^+|^2} = \sum_{\ell=0}^k \frac{1}{|\lambda^+ + \gamma\phi_\ell|^2} \left\| \sum_{w \in W} u(w)P_\ell|w\rangle \right\|^2.$$

We still have the problem of finding c^+ instead of the absolute value of c^+ . What we have to do is to rescale $|\lambda^+\rangle$ with a unit complex number $|\lambda^+\rangle \rightarrow e^{i\theta}|\lambda^+\rangle$ so that $c^+e^{-i\theta}$ is a positive real number. After calculating c^+ and $|u\rangle$, we are able to find $|\langle w|\lambda^+\rangle|$ because $\langle w|\lambda^+\rangle = c^+u(w)$.

The last missing quantity is $|\langle \lambda^+|\psi(0)\rangle|$. If graph $G(V, E)$ is regular and connected, the uniform superposition is an eigenvector of $\exp(-i\gamma A)$ and $\exp(-i\gamma\phi_0)$ is the eigenvalue, where ϕ_0 is the graph degree, with multiplicity one. In this case, using Eq. (4) taking $\ell = 0$ we obtain

$$\langle \psi(0)|\lambda^+\rangle = -\frac{1}{\lambda^+ + \gamma\phi_0} \sum_{w \in W} \langle w|\lambda^+\rangle \langle \psi(0)|w\rangle.$$

Since all terms on the right-hand side are supposedly known, this means that we have a recipe to calculate $|\langle \lambda^+|\psi(0)\rangle|$ if $G(V, E)$ is regular. If $G(V, E)$ is not regular, we take the initial state $|\psi(0)\rangle$ as an eigenvector of $-\gamma A$ associated with the largest eigenvalue of A . In this case, we also use Eq. (4) to obtain $\langle \psi(0)|\lambda^+\rangle$ in terms of known quantities.

The most straightforward extension of the method outlined above is to replace Eq. (7) by $\lambda^+ = -\gamma\phi_0 + \epsilon_1 + o(\epsilon_1)$ and $\lambda^- = -\gamma\phi_0 - \epsilon_2 + o(\epsilon_2)$, where $\epsilon_1 \neq \epsilon_2(1 + o(1))$. The asymptotic analysis is performed assuming that ϵ_1 and ϵ_2 tend to zero when the number of vertices increases. This extension may include the cases in which the dynamical evolution in the asymptotic limit depends on eigenvectors different from the ground state and the first excited state. The probability of finding a marked vertex as a function of t may not be the square of a sinusoidal function, such as $a^2 \sin^2 et$, but instead something like $a^2 + b^2 \sin^2 t(\epsilon_1 + \epsilon_2)/2$, from which we obtain the optimal running time $t = \pi/(\epsilon_1 + \epsilon_2)$ and $p_{\text{succ}} = a^2 + b^2$.

3 Johnson graphs

For the rest of this paper, we apply the general recipe given in the previous Section to the *Johnson graph* $G(V, E) = J(n, k)$. The vertex set V is the set of k -subsets of $[n] = \{1, 2, \dots, n\}$,

and two vertices $v, v' \in V$ are adjacent if and only if $|v \cap v'| = k - 1$. Note that $J(n, 1)$ is the complete graph K_n , and that $J(n, 2)$ is the triangular graph T_n , which is strongly regular. We will assume that $W = \{w_1, w_2\}$, where we fix k and let $n \rightarrow \infty$. In this case, the matrix M^λ from Eq. (6) is a two-dimensional matrix denoted by

$$M^\lambda = \begin{bmatrix} m_1 & m_3 \\ m_3 & m_2 \end{bmatrix},$$

where

$$\begin{aligned} m_1 &= \sum_{\ell=0}^k \frac{\|P_\ell|w_1\rangle\|^2}{\lambda + \gamma\phi_\ell} + 1, \\ m_2 &= \sum_{\ell=0}^k \frac{\|P_\ell|w_2\rangle\|^2}{\lambda + \gamma\phi_\ell} + 1, \\ m_3 &= \sum_{\ell=0}^k \frac{\langle w_1|P_\ell|w_2\rangle}{\lambda + \gamma\phi_\ell}. \end{aligned}$$

The eigenvalues λ of H are obtained from $\det(M^\lambda) = m_1 m_2 - m_3^2 = 0$.

The number of vertices of $J(n, k)$ is $N = \binom{n}{k}$. The $k + 1$ distinct eigenvalues $\phi_0 > \phi_1 > \dots > \phi_k$ of $J(n, k)$ are given by

$$\phi_\ell = (k - \ell)(n - k - \ell) - \ell, \quad (12)$$

and the multiplicity of ϕ_ℓ is $\binom{n}{\ell} - \binom{n}{\ell-1}$ (with the convention that $\binom{n}{-1} = 0$). See [36, 37, 38]. For the Johnson graph $J(n, k)$, it is important to remark that P_ℓ has constant diagonal entries $(\binom{n}{\ell} - \binom{n}{\ell-1})/\binom{n}{k}$, so that

$$\|P_\ell|w_1\rangle\|^2 = \|P_\ell|w_2\rangle\|^2 = \frac{\binom{n}{\ell} - \binom{n}{\ell-1}}{\binom{n}{k}} = \frac{k!(n-k)!(n-2\ell+1)}{\ell!(n-\ell+1)!}. \quad (13)$$

In particular, we have $m_1 = m_2$. Let

$$\delta = k - |w_1 \cap w_2|,$$

which is the distance between w_1 and w_2 . We note that m_3 depends on δ . More specifically, it is known that $\langle w_1|P_\ell|w_2\rangle$ is written in terms of a terminating ${}_3F_2$ hypergeometric series:

$$\langle w_1|P_\ell|w_2\rangle = \|P_\ell|w_1\rangle\|^2 {}_3F_2\left(\begin{matrix} -\ell, -\delta, \ell - n - 1 \\ k - n, -k \end{matrix} \middle| 1\right). \quad (14)$$

See, e.g., [36, pp. 219–220] and [39, Example 2.3]. From now on, we assume that δ is known in advance. After analyzing the search algorithm under this assumption, we will discuss the unrestricted case, in which δ is unknown.

3.1 An invariant subspace

For the single-marked case discussed in [34], a $(k + 1)$ -dimensional invariant subspace of \mathcal{H} played an important role. For the present case, we can again make use of a similar but more

complicated invariant subspace. For integers a, b, c such that $0 \leq a \leq k - \delta$, $a \leq b \leq c$, and $2k - n + \delta + a - b \leq c \leq \min\{k + a - b, \delta + a\}$, let

$$\nu_{a,b,c} = \{v \in V : |v \cap w_1 \cap w_2| = a, \{|v \cap w_1|, |v \cap w_2|\} = \{b, c\}\},$$

and set

$$|\nu_{a,b,c}\rangle = \sum_{v \in \nu_{a,b,c}} |v\rangle.$$

Then these (unnormalized) vectors $|\nu_{a,b,c}\rangle$ span an invariant subspace \mathcal{H}_{inv} of \mathcal{H} . This can be shown manually, but the group-theoretic interpretation is as follows. When $n > 2k$, the automorphism group of $J(n, k)$ is isomorphic to the symmetric group \mathfrak{S}_n on n letters $[n] = \{1, 2, \dots, n\}$. Consider the subgroup \mathfrak{G} of \mathfrak{S}_n consisting of the elements that fix W setwise. The elements of \mathfrak{G} fix each of the sets $w_1 \cap w_2$ and $[n] \setminus (w_1 \cup w_2)$, and either fix or swap the two sets $w_1 \setminus w_2$ and $w_2 \setminus w_1$. Hence, the order of \mathfrak{G} is $|\mathfrak{G}| = (k - \delta)! \times (n - k - \delta)! \times (\delta!)^2 \times 2$. The $\nu_{a,b,c}$ are the orbits of \mathfrak{G} on the vertex set V , and hence give rise to an invariant subspace. Indeed, since $Ag = gA$ for every $g \in \mathfrak{S}_n$, we have

$$A|\nu_{a,b,c}\rangle = A \cdot \frac{1}{|\mathfrak{G}|} \sum_{g \in \mathfrak{G}} g|\nu_{a,b,c}\rangle = \frac{1}{|\mathfrak{G}|} \sum_{g \in \mathfrak{G}} g(A|\nu_{a,b,c}\rangle),$$

and the right-hand side is invariant under \mathfrak{G} and thus written in the form $\sum_{a',b',c'} \kappa_{a',b',c'} |\nu_{a',b',c'}\rangle$ for some scalars $\kappa_{a',b',c'}$. Moreover, since $W = \nu_{k-\delta, k-\delta, k}$, we have

$$\left(\sum_{w \in W} |w\rangle\langle w| \right) |\nu_{a,b,c}\rangle = \delta_{k-\delta, a} \delta_{k-\delta, b} \delta_{k, c} |\nu_{k-\delta, k-\delta, k}\rangle.$$

Hence, it follows that \mathcal{H}_{inv} is invariant under H and thus also e^{-iHt} . Note also that the sum of the $|\nu_{a,b,c}\rangle$ equals $\sqrt{N}|\psi(0)\rangle$, so that $|\psi(0)\rangle$ belongs to \mathcal{H}_{inv} .

From now on, we will always consider eigenvectors $|\lambda\rangle$ in \mathcal{H}_{inv} . This assumption provides us with the following strong constraint:

$$\langle w_1 | \lambda \rangle = \langle w_2 | \lambda \rangle = \frac{\langle \nu_{k-\delta, k-\delta, k} | \lambda \rangle}{2}.$$

For the rest of this Section, let us call this common value α . The following is a strengthening of Proposition 1 in this case.

Proposition 3. *The following are equivalent: (i) $\lambda \in \sigma(-\gamma A)$; (ii) $-\gamma A|\lambda\rangle = \lambda|\lambda\rangle$; (iii) $\alpha = 0$.*

Proof. (iii) \Rightarrow (ii): Note that $-\gamma A|\lambda\rangle = H|\lambda\rangle = \lambda|\lambda\rangle$ by the definition of H .

(ii) \Rightarrow (i): Clear.

(i) \Rightarrow (iii): Suppose that $\lambda = -\gamma\phi_\ell$. Then, by Eq. (3), we have

$$\alpha (P_\ell |w_1\rangle + P_\ell |w_2\rangle) = 0,$$

where we note that $P_\ell A = AP_\ell = \phi_\ell P_\ell$. If $\ell = 0$ then $P_0 |w_1\rangle = P_0 |w_2\rangle = (1/\sqrt{N})|\psi(0)\rangle$, so $\alpha = 0$. If $\ell > 0$ then it follows from the fact that $J(n, k)$ is a primitive¹ distance-regular graph (provided $n > 2k$) that $P_\ell |w_1\rangle$ and $P_\ell |w_2\rangle$ are linearly independent (cf. [37, Sec. 9.1], [36, p. 137]), so again we have $\alpha = 0$, whence (iii). \square

¹A distance-regular graph with diameter k is called *primitive* if all the distance- i graphs ($i = 1, 2, \dots, k$) are connected.

Corollary 4. $-\gamma\phi_0$ is not an eigenvalue of H on \mathcal{H}_{inv} .

Proof. If $\lambda = -\gamma\phi_0$ then $|\psi(0)\rangle$ and $|\lambda\rangle$ are linearly independent eigenvectors of A with eigenvalue ϕ_0 . (The linear independence follows from $\langle w_1|\psi(0)\rangle = \langle w_2|\psi(0)\rangle = 1/\sqrt{N} \neq 0$ and $\alpha = 0$.) But ϕ_0 has multiplicity one since $J(n, k)$ is connected, a contradiction. \square

Corollary 5. Suppose that $\lambda \notin \sigma(-\gamma A)$. Then we have $m_1 + m_3 (= m_2 + m_3) = 0$.

Proof. Immediate from Eq. (5) and $\langle w_1|\lambda\rangle = \langle w_2|\lambda\rangle = \alpha \neq 0$. \square

This corollary simplifies the discussions of the calculations of λ^\pm because we can forget about the case where $m_1 - m_3 = 0$, which results in a “bad” (but putative) eigenvalue. We also note that the results of this Subsection can be generalized to other families of distance-transitive graphs, such as the Hamming graphs.

3.2 Calculation of λ^\pm and related quantities

First, we find the eigenvalue λ^- of the ground state of H . Note that the adjacency matrix A and the oracle $\sum_{w \in W} |w\rangle\langle w|$ are both nonnegative matrices with respect to the computational basis, and hence so are their matrix representations with respect to the $|\nu_{a,b,c}\rangle$ on \mathcal{H}_{inv} . Since $\gamma > 0$, it follows from the Perron–Frobenius theorem (see, e.g., [37, Sec. 3.1], [40, Sec. 2.2]) that the eigenvalue λ^- is in the interval $(-\infty, -\gamma\phi_0)$ and has multiplicity one. Moreover, observe that $m_1 + m_3$, as a function of λ , is monotone decreasing on $(-\infty, -\gamma\phi_0)$ since $|\langle w_1|P_\ell|w_2\rangle| \leq \|P_\ell|w_1\rangle\|^2 = \|P_\ell|w_2\rangle\|^2$ by the Cauchy–Schwarz inequality and Eq. (13). Hence, it follows from Corollary 5 that λ^- is the *unique* eigenvalue of H on \mathcal{H}_{inv} in $(-\infty, -\gamma\phi_0)$.

We write

$$\begin{aligned} S_1 &= S_{w_1 w_1}^{(1)} = S_{w_2 w_2}^{(1)}, & S'_1 &= S_{w_1 w_2}^{(1)} = S_{w_2 w_1}^{(1)}, \\ S_2 &= S_{w_1 w_1}^{(2)} = S_{w_2 w_2}^{(2)}, & S'_2 &= S_{w_1 w_2}^{(2)} = S_{w_2 w_1}^{(2)}, \end{aligned}$$

and

$$\lambda = -\gamma\phi_0 + \epsilon.$$

We choose γ so that $\epsilon(m_1 + m_2)$ has no linear term in ϵ , i.e.,

$$\gamma = S_1 + S'_1. \tag{15}$$

We note that S'_1 depends on the distance δ , which we currently assume is known in advance.

To proceed with the calculations, we need the following expressions for the sums S_1, S_2, S'_1 , and S'_2 :

$$S_1 = \frac{1}{kn} + O\left(\frac{1}{n^2}\right), \quad S_2 = \frac{1}{k^2 n^2} + O\left(\frac{1}{n^3}\right), \tag{16}$$

$$S'_1 = O\left(\frac{1}{n^{\delta+1}}\right), \quad S'_2 = O\left(\frac{1}{n^{\delta+2}}\right). \tag{17}$$

Eq. (16) follows easily from Eqs. (12) and (13). The proof of Eq. (17) is deferred to Appendix A. From Eqs. (16) and (17) it follows that

$$\gamma = \frac{1}{kn} + O\left(\frac{1}{n^2}\right). \tag{18}$$

For convenience, set

$$\eta = \frac{1}{n}.$$

By Eq. (13), we have

$$\|P_\ell|w_1\rangle\|^2 = \frac{k!\eta^{k-\ell}(1-(2\ell-1)\eta)}{\ell!(1-(\ell-1)\eta)\cdots(1-(k-1)\eta)} \quad (0 \leq \ell \leq k),$$

which is analytic around $\eta = 0$. Moreover, it follows from Eq. (14) that $\langle w_1|P_\ell|w_2\rangle$ is also analytic around $\eta = 0$. By Eqs. (12) and (18), we have

$$\gamma(\phi_0 - \phi_\ell) = \frac{\ell}{k} + O(\eta) \quad (1 \leq \ell \leq k), \quad (19)$$

and this is also analytic around $\eta = 0$. Since the constant term of the right-hand side is nonzero, it follows from the above comments that $\epsilon(m_1 + m_3)$, as a bivariate function of η and $\epsilon = \lambda + \gamma\phi_0$, is analytic around the origin $(\eta, \epsilon) = (0, 0)$. Hence, the power series expansion of $\epsilon(m_1 + m_3)$ centered at the origin converges absolutely and uniformly on some neighborhood of the origin (see [41, Sec. 2.3]), and expressed in the form

$$\epsilon(m_1 + m_3) = \frac{2}{N} - \frac{S_2 + S'_2}{\gamma^2} \epsilon^2 + O(\epsilon^3)$$

with respect to ϵ , where we recall that the linear term in ϵ vanishes, and that

$$\frac{2}{N} = 2k!\eta^k + O(\eta^{k+1}), \quad \frac{S_2 + S'_2}{\gamma^2} = 1 + o(1)$$

by Eqs. (16) and (17). We note that the expression $O(\epsilon^3)$ in the above expansion is evaluated uniformly in η on this neighborhood. Now, set

$$\epsilon_0^- = -\frac{\sqrt{2}\gamma}{\sqrt{N(S_2 + S'_2)}} = -\frac{\sqrt{2}}{\sqrt{N}}(1 + o(1)).$$

Pick any scalar $\nu \in (1, 2)$, and let $c \in (0, 1)$ be such that $O(\epsilon^3)$ above is bounded as

$$|O(\epsilon^3)| < |\epsilon|^{1+\nu} 2^{-\nu}$$

for every $\epsilon \in (-c, c)$. Let n be large enough so that $|\epsilon_0^-| < c/2$ and $(S_2 + S'_2)/\gamma^2 > 2/3$. Then $\epsilon_0^- \pm |\epsilon_0^-|^\nu \in (-c, c)$ and we have

$$\begin{aligned} |O((\epsilon_0^- \pm |\epsilon_0^-|^\nu)^3)| &< |\epsilon_0^- \pm |\epsilon_0^-|^\nu|^{1+\nu} 2^{-\nu} \\ &< |\epsilon_0^-|^\nu |\epsilon_0^- \pm |\epsilon_0^-|^\nu| \\ &< |\epsilon_0^-|^\nu |2\epsilon_0^- \pm |\epsilon_0^-|^\nu| \cdot \frac{2}{3} \\ &< \frac{S_2 + S'_2}{\gamma^2} |\epsilon_0^-|^\nu |2\epsilon_0^- \pm |\epsilon_0^-|^\nu|. \end{aligned}$$

Note that the right-hand side equals the absolute value of $2/N - (S_2 + S'_2)\epsilon^2/\gamma^2$ for $\epsilon = \epsilon_0^- \pm |\epsilon_0^-|^\nu$. Hence, for such large n , we have $\epsilon(m_1 + m_3) < 0$ for $\epsilon = \epsilon_0^- - |\epsilon_0^-|^\nu$ and $\epsilon(m_1 + m_3) > 0$ for $\epsilon =$

$\epsilon_0^- + |\epsilon_0^-|^\nu$. By the mean value theorem, this shows that there exists $\epsilon^- \in (\epsilon_0^- - |\epsilon_0^-|^\nu, \epsilon_0^- + |\epsilon_0^-|^\nu)$ such that $m_1 + m_3 = 0$ for $\epsilon = \epsilon^-$. In view of our previous comments, such ϵ^- is unique and we must have

$$\lambda^- = -\gamma\phi_0 + \epsilon^-.$$

This also establishes

$$\epsilon^- = -\frac{\sqrt{2}}{\sqrt{N}}(1 + o(1)). \quad (20)$$

Recall the scalar $\alpha = \alpha^-$ for the eigenvalue λ^- , which is nonzero by Proposition 3. We assume that $\alpha^- > 0$ after a rescaling of $|\lambda^- \rangle$. By Eq. (4) and $\sum_{\ell=0}^k \|P_\ell |\lambda^- \rangle\|^2 = 1$, we routinely obtain

$$1 = (\alpha^-)^2 \left(\frac{4}{N(\epsilon^-)^2} + 2(S_2 + S_2') + O(\epsilon^-) \right),$$

so that from Eqs. (16), (17), and (20) it follows that

$$\alpha^- = \frac{1}{2} + o(1). \quad (21)$$

Recall that $|\psi(0)\rangle$ is a ϕ_0 -eigenvector of A . By Eq. (4) with $\ell = 0$, we also obtain

$$\langle \psi(0) | \lambda^- \rangle = -\frac{2\alpha^-}{\sqrt{N}\epsilon^-} = \frac{1}{\sqrt{2}} + o(1), \quad (22)$$

where we have also used Eqs. (20) and (21).

We next find the eigenvalue λ^+ for the first excited state of H . On the one hand, by the definition of H and $|\psi(0)\rangle$, we have

$$\langle \psi(0) | H | \psi(0) \rangle = -\gamma\phi_0 - \frac{1}{N}.$$

On the other hand, we also have

$$\langle \psi(0) | H | \psi(0) \rangle = \lambda^- |\langle \psi(0) | \lambda^- \rangle|^2 + \sum_{\lambda \neq \lambda^-} \lambda |\langle \psi(0) | \lambda \rangle|^2,$$

where the sum on the right-hand side is over the eigenvalues of H on \mathcal{H}_{inv} other than λ^- . By Eqs. (20) and (22), we have

$$\lambda^- |\langle \psi(0) | \lambda^- \rangle|^2 = -\frac{\gamma\phi_0}{2} + o(1).$$

Suppose now that $\lambda^+ \geq -\gamma\phi_1$. Then, since $\sum_{\lambda} |\langle \psi(0) | \lambda \rangle|^2 = 1$, it follows from Eqs. (19) with $\ell = 1$ and (22) that

$$\sum_{\lambda \neq \lambda^-} \lambda |\langle \psi(0) | \lambda \rangle|^2 \geq -\gamma\phi_1 \sum_{\lambda \neq \lambda^-} |\langle \psi(0) | \lambda \rangle|^2 = -\frac{\gamma\phi_1}{2} + o(1) = -\frac{\gamma\phi_0}{2} + \frac{1}{2k} + o(1).$$

However, this implies that

$$\langle \psi(0) | H | \psi(0) \rangle \geq -\gamma\phi_0 + \frac{1}{2k} + o(1) > -\gamma\phi_0 - \frac{1}{N}$$

for large n , which is a contradiction. (Recall that k is fixed.) Hence, for large n , it follows that $\lambda^+ < -\gamma\phi_1$ and thus $\lambda^+ \in (-\gamma\phi_0, -\gamma\phi_1)$ by virtue of Corollary 4. Observe that $m_1 + m_3$ (again as a function of λ) is also monotone decreasing on $(-\gamma\phi_0, -\gamma\phi_1)$, from which it follows that λ^+ is the *unique* eigenvalue of H on \mathcal{H}_{inv} in this range. We may now proceed as in the above discussions, and conclude that

$$\lambda^+ = -\gamma\phi_0 + \epsilon^+,$$

where

$$\epsilon^+ = \frac{\sqrt{2}}{\sqrt{N}}(1 + o(1)).$$

We also obtain the scalar $\alpha = \alpha^+$ for the eigenvalue λ^+ as

$$\alpha^+ = \frac{1}{2} + o(1), \tag{23}$$

and

$$\langle \psi(0) | \lambda^+ \rangle = -\frac{2\alpha^+}{\sqrt{N}\epsilon^+} = -\frac{1}{\sqrt{2}} + o(1). \tag{24}$$

3.3 Computational complexity

Now we apply the general recipe outlined in the previous Section to the search algorithm on $J(n, k)$ by fixing k and letting $n \rightarrow \infty$. Using Eqs. (21), (22), (23), and (24), we check that the condition (8) is true. The probability of finding a marked vertex as a function of time is given by Eq. (9) and then using Eq. (10) the optimal running time is

$$t_{\text{run}} = \frac{\pi\sqrt{N}}{2\sqrt{2}},$$

and using Eq. (11) the success probability is

$$p_{\text{succ}} = 1 + o(1). \tag{25}$$

Note that the asymptotic success probability does not depend on δ , the distance between the two marked vertices w_1 and w_2 .

We have so far assumed that δ is known in advance; see Eq. (15). In the case where we have no prior information on δ , we simply apply the above search algorithm in turn for $\delta = 1, 2, \dots, k$. We note that we can check if the outcome is a marked vertex by applying the oracle for each of the k steps. Hence, the success probability is still given by Eq. (25). The running time is at most

$$\frac{\pi k \sqrt{N}}{2\sqrt{2}}.$$

We fix k , so this is still of order $O(\sqrt{N})$.

4 Final remarks

We have described a framework to determine the computational complexity of spatial search algorithms by continuous-time quantum walk on graphs with multiple marked vertices. The

framework is successful if the evolution operator satisfies a few properties. The most important one is that the dynamical evolution in the asymptotic limit depends only on two eigenvectors of the Hamiltonian, the ground state and the first excited state, which are associated with the smallest eigenvalues. The optimal running time depends only on the spectral gap in this case. To find the spectrum of the Hamiltonian and the success probability, we need to know in advance the eigenvalues and eigenvectors of the adjacency matrix. The simplest cases have a success probability that is described by the square of a sinusoidal function $a^2 \sin^2 \epsilon t$, where 2ϵ is the spectral gap. The optimal running time is given by $t = \pi/2\epsilon$ and then the success probability is $p_{\text{succ}} = a^2$. We have given directions on how to address the cases in which the dynamical evolution in the asymptotic limit depends on eigenvectors different from the ground state and the first excited state.

To show an example of our framework, we have analyzed the spatial search algorithm by continuous-time quantum walk on the Johnson graph $J(n, k)$ with two marked vertices. We have shown that the optimal running time in this case is $\pi\sqrt{N}/2\sqrt{2}$, where N is the number of vertices, when k is fixed and the distance δ between the marked vertices is known in advance. When we do not know δ , we have to repeat the algorithm k times assuming all possible values of δ . The total running time is at most $\pi k\sqrt{N}/2\sqrt{2}$ with success probability $1 + o(1)$ when $n \rightarrow \infty$.

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Appendix

A The proof of Eq. (17)

We first invoke some results from [42] to evaluate the ${}_3F_2$ series in Eq. (14). Set

$$\phi_\ell = \phi_0 + h\ell(\ell + 1 + s), \quad \phi_\ell^* = \phi_0^* + s^*\ell$$

for $0 \leq \ell \leq k$, and

$$\alpha_\ell = hs^*\ell(\ell - k - 1)(\ell + r), \quad \beta_\ell = hs^*\ell(\ell - k - 1)(\ell + r - s - k - 1)$$

for $1 \leq \ell \leq k$, where

$$s = -n - 2, \quad r = k - n - 1,$$

and ϕ_0, ϕ_0^*, h , and s^* are arbitrary with $h, s^* \neq 0$. The sequence

$$(\phi_\ell, \phi_\ell^*, \ell = 0, \dots, k; \alpha_{\ell'}, \beta_{\ell'}, \ell' = 1, \dots, k)$$

is a *parameter array* of dual Hahn type; cf. [42, Example 5.12]. Note that the ϕ_ℓ agree with the eigenvalues of $J(n, k)$ (cf. Eq. (12)) provided that we set $\phi_0 = k(n - k)$ and $h = 1$. Moreover, we have

$${}_3F_2 \left(\begin{matrix} -\ell, -\delta, \ell - n - 1 \\ k - n, -k \end{matrix} \middle| 1 \right) = f_\delta(\phi_\ell),$$

where

$$f_\delta(x) = \sum_{\nu=0}^{\delta} \frac{(x - \phi_0) \cdots (x - \phi_{\nu-1})(\phi_\delta^* - \phi_0^*) \cdots (\phi_\delta^* - \phi_{\nu-1}^*)}{\alpha_1 \cdots \alpha_\nu}.$$

By [42, Theorem 4.1, Lemma 4.2], we have

$$f_\delta(x) = \frac{\beta_1 \cdots \beta_\delta}{\alpha_1 \cdots \alpha_\delta} f_\delta^\Downarrow(x) = \frac{\delta!}{(k-n)_\delta} f_\delta^\Downarrow(x),$$

where

$$f_\delta^\Downarrow(x) = \sum_{\nu=0}^{\delta} \frac{(x - \phi_k) \cdots (x - \phi_{k-\nu+1})(\phi_\delta^* - \phi_0^*) \cdots (\phi_\delta^* - \phi_{\nu-1}^*)}{\beta_1 \cdots \beta_\nu},$$

and $(a)_m = a(a+1) \cdots (a+m-1)$ denotes the shifted factorial. We have

$$f_\delta^\Downarrow(\phi_\ell) = {}_3F_2 \left(\begin{matrix} \ell - k, -\delta, n - k - \ell + 1 \\ 1, -k \end{matrix} \middle| 1 \right),$$

and hence

$${}_3F_2 \left(\begin{matrix} -\ell, -\delta, \ell - n - 1 \\ k - n, -k \end{matrix} \middle| 1 \right) = \frac{\delta!}{(k-n)_\delta} {}_3F_2 \left(\begin{matrix} \ell - k, -\delta, n - k - \ell + 1 \\ 1, -k \end{matrix} \middle| 1 \right). \quad (26)$$

By Eqs. (12), (13), (14), and (26), we have

$$\frac{\langle w_1 | P_\ell | w_2 \rangle}{\phi_0 - \phi_\ell} = O\left(\frac{1}{n^{k-\ell+1+\delta-\tau}}\right), \quad \frac{\langle w_1 | P_\ell | w_2 \rangle}{(\phi_0 - \phi_\ell)^2} = O\left(\frac{1}{n^{k-\ell+2+\delta-\tau}}\right)$$

for $1 \leq \ell \leq k$, where $\tau = \min\{k - \ell, \delta\}$, and Eq. (17) follows.

We remark that the above method can be generalized to other families of Q -polynomial distance-regular graphs, again including the Hamming graphs (see [37, Chap. 9]).

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