

Finding structural anomalies in graphs by means of quantum walks

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We explore the possibility of using quantum walks on graphs to find structural anomalies, such as extra edges or loops, on a graph. We focus our attention on star graphs, whose edges are like spokes coming out of a central hub. If there are N spokes, we show that a quantum walk can find an extra edge connecting two of the spokes or a spoke with a loop on it in $O(\sqrt{N})$ steps. We initially find that if all except one of the spokes have loops, the walk will not find the spoke without a loop, but this can be fixed if we choose the phase with which the particle is reflected from the vertex without the loop. Consequently, quantum walks can, under some circumstances, be used to find structural anomalies in graphs.

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A quantum walk is a quantum version of a random walk [1]. Both types of walks occur on a graph, which is a set of vertices connected by edges. A particle making a quantum walk behaves differently from one making a classical random walk because the mathematical objects that govern its motion are amplitudes rather than probabilities, which means that interference effects play a role. There are two basic types of quantum walk: one in which time progresses in discrete steps [2] and the other in which time is continuous [3]. Here we are concerned with a particular version of the discrete-time walk known as the scattering quantum walk [4]. In this type of quantum walk, the particle resides on the edges and scatters at the vertices at each time step. Recently, considerable experimental progress on implementing quantum walks has been made [5–10], and a recent review of the entire subject can be found in Ref. [11].

Quantum walks have been used to develop quantum algorithms, and this had proven to be a fruitful approach [12–15]. They were first used to conduct searches on graphs [16–19]. In a quantum walk search, the properties of one of the vertices differ from those of the others, often by doing what the other vertices do but adding a sign flip, which marks that vertex. The object of the search is to find the marked vertex. Quantum walk searches have been explored on a number of types of graphs, including hypercubes, grids, and complete graphs. Recently, it has also been shown that quantum walks can find marked edges and a marked complete subgraph of a complete graph [20]. Here we would like to explore a different question: whether quantum walks can find structural anomalies in graphs. We look in some detail at the problem of finding an extra edge in a particular type of graph, and then we present results on finding other types of anomalous elements.

We consider what we call a star graph (see Fig. 1). This graph has a high degree of symmetry, which means that analyzing walks on it becomes relatively simple because the Hilbert space in which the walk occurs is of relatively small dimension [19,21]. This graph has a central vertex, which we label 0, and N additional vertices, which we label 1 through N . The central vertex is connected to each of the other vertices by an edge, and, for now, the vertices 1, 2, . . . , N are not connected

to each other by edges. In order to construct a quantum walk on this graph we first need a Hilbert space for the particle making the walk. We specify this by means of an orthonormal basis consisting of the states $\{|0, j\rangle, |j, 0\rangle | j = 1, 2, \dots, N\}$. The state $|0, j\rangle$ corresponds to the particle being on the edge between 0 and j going from 0 to j , and the state $|j, 0\rangle$ corresponds to the particle again being on the edge between 0 and j , but now going from j to 0. Next we need a unitary operator that advances the walk by one time step. That is provided by the collective action of unitaries at each vertex that tell how the particle scatters as it passes through that vertex. If U is the unitary that advances the walk one step, it acts on a particle entering the vertex 0 as

$$U|j, 0\rangle = -r|0, j\rangle + t \sum_{k=1, k \neq j}^N |0, k\rangle, \quad (1)$$

where $r = (N - 2)/N$ and $t = 2/N$. That is, the particle has an amplitude of $-r$ of being reflected and an amplitude t of being transmitted to one of the other edges. We now need to choose what happens at vertices 1 through N . If we make the choice $U|0, j\rangle = |j, 0\rangle$ for $j > 1$ and $U|0, 1\rangle = -|1, 0\rangle$, we obtain an implementation of the Grover search algorithm. Starting with an equal superposition of all of the basis states, after $O(\sqrt{N})$ steps, the particle will be located on the edge connecting vertices 0 and 1.

Here we wish to do something different. First, we add an edge between vertices 1 and 2. The unitary operator now acts as $U|0, j\rangle = |j, 0\rangle$ for $j > 2$, and

$$\begin{aligned} U|0, 1\rangle &= |1, 2\rangle, & U|0, 2\rangle &= |2, 1\rangle, \\ U|1, 2\rangle &= |2, 0\rangle, & U|2, 1\rangle &= |1, 0\rangle. \end{aligned} \quad (2)$$

Note that we have assumed that vertices 1 and 2 transmit the particle, and there is no reflection. One can put in an amplitude for reflection, but, if it is not too large, this does not change our results appreciably. The walk resulting from this choice of U can be analyzed easily, because it stays within a

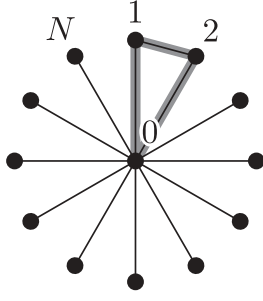


FIG. 1. Star graph with an extra edge between vertices 1 and 2.

five-dimensional subspace of the entire Hilbert space. Define the states

$$\begin{aligned}
 |\psi_1\rangle &= \frac{1}{\sqrt{2}}(|0,1\rangle + |0,2\rangle), \\
 |\psi_2\rangle &= \frac{1}{\sqrt{2}}(|1,0\rangle + |2,0\rangle), \\
 |\psi_3\rangle &= \frac{1}{\sqrt{N-2}} \sum_{j=3}^N |0,j\rangle, \\
 |\psi_4\rangle &= \frac{1}{\sqrt{N-2}} \sum_{j=3}^N |j,0\rangle, \\
 |\psi_5\rangle &= \frac{1}{\sqrt{2}}(|1,2\rangle + |2,1\rangle).
 \end{aligned} \quad (3)$$

These states span a five-dimensional space we call S . The unitary transformation U that advances the walk one step acts on these states as follows:

$$\begin{aligned}
 U|\psi_1\rangle &= |\psi_5\rangle, \\
 U|\psi_2\rangle &= -(r-t)|\psi_1\rangle + 2\sqrt{rt}|\psi_3\rangle, \\
 U|\psi_3\rangle &= |\psi_4\rangle, \\
 U|\psi_4\rangle &= (r-t)|\psi_3\rangle + 2\sqrt{rt}|\psi_1\rangle, \\
 U|\psi_5\rangle &= |\psi_2\rangle.
 \end{aligned} \quad (4)$$

For our initial state we choose

$$\begin{aligned}
 |\psi_{\text{init}}\rangle &= \frac{1}{\sqrt{2N}} \sum_{j=1}^N (|0,j\rangle - |j,0\rangle) = \frac{1}{\sqrt{N}}(|\psi_1\rangle - |\psi_2\rangle) \\
 &+ \sqrt{\frac{N-2}{2N}}(|\psi_3\rangle - |\psi_4\rangle),
 \end{aligned} \quad (5)$$

which is in S . Since the initial state is in S , and S is an invariant subspace of U , the entire walk will remain in S , and this reduces the complexity of our problem considerably. We should mention that the minus sign in the first expression for initial state is essential; if it is replaced by a plus sign, the search will fail.

In order to find the evolution of the quantum state for the walk, we find the eigenvalues and eigenstates of U restricted to S . This gives us the spectral representation of U and makes finding U^n , the operator that advances the walk n steps,

straightforward. We then find that, to good approximation assuming that N is large,

$$U^n |\psi_{\text{init}}\rangle = \frac{(-1)^n}{\sqrt{3}} \begin{pmatrix} \sin(n\Delta) \\ \sin(n\Delta) \\ \sqrt{3/2} \cos(n\Delta) \\ -\sqrt{3/2} \cos(n\Delta) \\ -\sin(n\Delta) \end{pmatrix}, \quad (6)$$

where the first entry is the coefficient of $|\psi_1\rangle$, the second is the coefficient of $|\psi_2\rangle$, and so on, and $\Delta = (2t/3)^{1/2}$. This is the state of the walk after n steps. From this equation, and the definitions of $|\psi_1\rangle$ through $|\psi_5\rangle$, we see that, when $n\Delta = \pi/2$, the particle is located on one of the edges leading to the extra edge or on the extra edge itself. This happens when $n = O(\sqrt{N})$.

We now need to discuss how to interpret this result. It is reasonable to assume that, if we are given a graph with an extra edge in an unknown location, we only have access to the edges connecting the central vertex to the outer ones and not to the extra edge itself. (If we had access to the extra edge, then we would have to know where it is.) That is, in making a measurement, we can only determine which of the edges connecting the central vertex to the outer ones the particle is on. If it is on the extra edge, we do not detect it. So, after n steps, where $n\Delta = \pi/2$, we measure the edges to which we have access to find out where the particle is. With probability $2/3$ it will be on an edge connected to the extra edge, and with probability $1/3$ it will be on the extra edge itself, in which case we do not detect it.

In comparing this procedure to a classical search for the extra edge, we assume that classically the graph is specified by an adjacency list, which is an efficient specification for sparse graphs. For each vertex of the graph, one lists the vertices that are connected to it by an edge. In our case, the central vertex is connected to all of the other vertices, the vertices not connected to the extra edge are connected only to the central vertex, and two of the outer vertices are connected to the central vertex and to each other. Searching this list classically would require $O(N)$ steps to find the extra edge, while the quantum procedure succeeds in $O(\sqrt{N})$.

One can ask whether other structural anomalies can be detected by means of a quantum walk. One possibility is to take the basic star graph and add a loop to one of the outer vertices, say vertex 1. If we call the state corresponding to the particle being on the loop $|l_1\rangle$, the unitary time-step operator would act on the states going into the outer vertices as $U|0,1\rangle = |l_1\rangle$, $U|l_1\rangle = |1,0\rangle$, and $U|0,j\rangle = |j,0\rangle$ for $j > 1$. The action of U for states going into the central vertex is as before. The details of the calculations for this walk will be presented elsewhere, but the result is similar to what we found in the case of the extra edge. Starting with the same initial state as before, if $n\sqrt{t/3} = \pi/2$, then with probability $2/3$ the particle will be on the edge connecting vertex 1 to the central vertex, and with probability $1/3$ it will be on the loop itself. Therefore, a quantum walk can be used to find the vertex with the loop attached in $O(\sqrt{N})$ steps.

A second possibility is simply to extend one of the edges. One adds an extra edge and an extra vertex, which we call

A. One end of this edge is attached to vertex 1, and the other to vertex A . Vertex A is connected only to vertex 1. The unitary time-step operator now acts on the states going into the outer vertices as $U|0,1\rangle = |1,A\rangle$, $U|1,A\rangle = |A,1\rangle$, $U|A,1\rangle = |1,0\rangle$, and $U|0,j\rangle = |j,0\rangle$ for $j > 1$. For an initial state, one chooses an arbitrary superposition of all of the states going out, $|\psi_{\text{out}}\rangle = (1/\sqrt{N})\sum_{j=1}^N |0,j\rangle$, and all of the states going in, $|\psi_{\text{in}}\rangle = (1/\sqrt{N})\sum_{j=1}^N |j,0\rangle$. For any initial state of this type, if one then runs a quantum walk on this graph, the particle does not become localized on the extra edge or on the edge leading to it in $O(\sqrt{N})$ steps. So, in this case, the quantum walk fails to find the structural anomaly with a quantum speedup.

Finally, let us see whether a quantum walk can find a missing element. Suppose we add loops to all of the outer vertices of our star graph except for one, say, as usual, vertex 1. We designate the loop state connected to vertex j by $|l_j\rangle$. The action of the unitary time-step operator on the outer vertices is now $U|0,1\rangle = |1,0\rangle$, and for $j > 1$, $U|0,j\rangle = |l_j\rangle$ and $U|l_j\rangle = |j,0\rangle$. As in the previous case, starting with a state that is an arbitrary superposition of the ingoing and outgoing states, we find that for no initial state of this type does the particle become localized on the edge without the loop in $O(\sqrt{N})$ steps, so the quantum walk again fails to find the anomaly with a quantum speedup.

These failures can be turned into successes, however, if we make a small modification to the walks. In the case of the extra edge, suppose that, instead of $U|1,A\rangle = |A,1\rangle$, we have $U|1,A\rangle = -|A,1\rangle$, with the action of U on all of the other states being the same as before. Then with an initial state that is an arbitrary superposition of $|\psi_{\text{out}}\rangle$ and $|\psi_{\text{in}}\rangle$, the particle will be localized on the extra edge and the edge leading to it in $O(\sqrt{N})$ steps. This situation is very much reminiscent of the standard Grover search.

The case of the missing loop is more interesting. Suppose that, instead of $U|0,1\rangle = |1,0\rangle$, we have $U|0,1\rangle = e^{i\phi}|1,0\rangle$. We find that the particle will be localized on the edge with the missing loop in $O(\sqrt{N})$ steps if $\phi = \pi, \pm(\pi/3)$, and if the initial state is properly chosen. In order to explain this last point, let us rephrase the problem slightly. We add a dummy loop to the vertex 1, $|l_1\rangle$ where $U|l_1\rangle = |l_1\rangle$, that does not participate in the dynamics (we still have $U|0,1\rangle = e^{i\phi}|1,0\rangle$). So our search problem becomes finding the vertex with the dummy loop. Define the state $|\psi_{\text{loop}}\rangle = (1/\sqrt{N})\sum_{j=1}^N |l_j\rangle$. Now, for the case $\phi = \pi$, we will have a successful quantum walk search; that is, the particle will become localized on the edge connected to the dummy loop in $O(\sqrt{N})$ steps, if we start in the state

$$|\psi_{\text{init}}\rangle = \frac{1}{\sqrt{3}}(|\psi_{\text{out}}\rangle + |\psi_{\text{in}}\rangle + |\psi_{\text{loop}}\rangle), \quad (7)$$

and in the case $\phi = \pi/3$ the proper initial state is

$$|\psi_{\text{init}}\rangle = \frac{1}{1 - e^{2\pi i/3}}(e^{-2\pi i/3}|\psi_{\text{out}}\rangle + |\psi_{\text{in}}\rangle + e^{2\pi i/3}|\psi_{\text{loop}}\rangle). \quad (8)$$

Therefore, by adjusting the phase on the edge with the dummy loop and choosing the proper initial state, the quantum walk can find the location of the dummy loop in $O(\sqrt{N})$ steps.

We have found that a successful quantum walk search on a modified star graph is associated with a degenerate eigenvalue of the unperturbed problem. The unperturbed evolution operator U_0 is obtained by setting $r = 1$ and $t = 0$ in matrix for U (this is the $N \rightarrow \infty$ limit of U). The perturbation, $\Delta U = U - U_0$, is small if N is large. If an eigenvalue of U_0 is simple, we have found that adding the perturbation adds a correction to it of order $1/N$, while if it is degenerate, adding ΔU removes the degeneracy, and one obtains corrections of order $1/\sqrt{N}$. Note that U^n can be expressed as

$$U^n = \sum_j \lambda_j^n P_j, \quad (9)$$

where λ_j is an eigenvalue of U and P_j is the projection onto the corresponding eigenvector. Because U is unitary, its eigenvalues have a magnitude of 1. Now suppose that $\lambda_j = \exp[i(\theta_j + \Delta\theta_j)]$, where $\exp(i\theta_j)$ is the corresponding eigenvalue of U_0 and $\exp(i\Delta\theta_j)$ is the correction due to ΔU . For the quantum search to succeed in $O(\sqrt{N})$ steps [i.e., $n = O(\sqrt{N})$], the effect of ΔU on the state, which is given by $\exp(in\Delta\theta_j)$, must be significant. This is true if $\Delta\theta_j = O(1/\sqrt{N})$ but not if $\Delta\theta_j = O(1/N)$.

In conclusion, we have shown that quantum walks can find structural anomalies in graphs, and not just marked elements. Here, only a few examples have been studied, so the question of what kinds of anomalies on what kinds of graphs can be efficiently found by means of a quantum walk is largely open. For example, it has been found that if one removes an edge from a complete graph, merely adjusting the reflection and transmission amplitudes of the affected vertices to maintain unitarity, a quantum walk will not efficiently find the missing edge [22]. This leads one to ask whether there are structural changes one can make in a complete graph that will be efficiently found in a quantum walk search. Questions such as this remain for the future. However, what we have found here suggests that the types of objects that can be found by a quantum walk search go beyond just marked vertices.

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- [1] Y. Aharonov, L. Davidovich, and N. Zagury, *Phys. Rev. A* **48**, 1687 (1993).
 [2] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, in *Proceedings of the Thirty-Third ACM Symposium on the*

Theory of Computing (Association for Computing Machinery, New York, 2001), pp. 50–59.

- [3] E. Farhi and S. Gutmann, *Phys. Rev. A* **58**, 915 (1998).

- [4] M. Hillery, J. Bergou, and E. Feldman, *Phys. Rev. A* **68**, 032314 (2003).
- [5] P. L. Knight, E. Roldán, and J. E. Sipe, *Phys. Rev. A* **68**, 020301 (2003).
- [6] D. Bouwmeester, I. Marzoli, G. P. Karman, W. Schleich, and J. P. Woerdman, *Phys. Rev. A* **61**, 013410 (1999).
- [7] H. B. Perets, Y. Lahini, F. Pozzi, M. Sorel, R. Morandotti, and Y. Silberberg, *Phys. Rev. Lett.* **100**, 170506 (2008).
- [8] H. Schmitz, R. Matjeschk, C. Schneider, J. Glueckert, M. Enderlein, T. Huber, and T. Schaetz, *Phys. Rev. Lett.* **103**, 090504 (2009).
- [9] M. Karski, L. Forster, J.-M. Choi, A. Steffen, W. Alt, D. Meschede, and A. Widera, *Science* **325**, 174 (2009).
- [10] A. Schreiber, K. N. Cassemiro, V. Potoček, A. Gabris, P. Mosley, E. Andersson, I. Jex, and Ch. Silberhorn, *Phys. Rev. Lett.* **104**, 050502 (2010).
- [11] V. Kendon, *Math. Struct. Comp. Sci.* **17**, 1169 (2007).
- [12] A. Ambainis, *SIAM J. Comput.* **37**, 210 (2007).
- [13] A. Childs and J. Eisenberg, *Quantum Inf. Comput.* **5**, 593 (2005).
- [14] A. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D. Spielman, in *Proceedings of the Thirty-Fifth ACM Symposium on the Theory of Computing* (Association for Computing Machinery, New York, 2003), pp. 59–68.
- [15] E. Farhi, J. Goldstone, and S. Gutmann, e-print [arXiv:quant-ph/0702144](https://arxiv.org/abs/quant-ph/0702144).
- [16] N. Shenvi, J. Kempe, and K. Birgitta Whaley, *Phys. Rev. A* **67**, 052307 (2003).
- [17] A. Ambainis, J. Kempe, and A. Rivosh, in *Proceedings of the 16th ACM-SIAM Symposium on Discrete Algorithms* (Society for Industrial and Applied Mathematics, Philadelphia, PA, 2005), pp. 1099–1108.
- [18] A. M. Childs and J. Goldstone, *Phys. Rev. A* **70**, 022314 (2004).
- [19] D. Reitzner, M. Hillery, E. Feldman, and V. Bužek, *Phys. Rev. A* **79**, 012323 (2009).
- [20] M. Hillery, D. Reitzner, and V. Bužek, *Phys. Rev. A* **81**, 062324 (2010).
- [21] H. Krovi and T. A. Brun, *Phys. Rev. A* **75**, 062332 (2007).
- [22] M. Hillery (unpublished).