Connectivity is a Poor Indicator of Fast Quantum Search

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A randomly walking quantum particle evolving by Schrödinger's equation searches on d-dimensional cubic lattices in $O(\sqrt{N})$ time when $d \ge 5$, and with progressively slower runtime as d decreases. This suggests that graph connectivity (including vertex, edge, algebraic, and normalized algebraic connectivities) is an indicator of fast quantum search, a belief supported by fast quantum search on complete graphs, strongly regular graphs, and hypercubes, all of which are highly connected. In this Letter, we show this intuition to be false by giving two examples of graphs for which the opposite holds true: one with low connectivity but fast search, and one with high connectivity but slow search. The second example is a novel two-stage quantum walk algorithm in which the walking rate must be adjusted to yield high search probability.

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Introduction.—Despite ten years elapsing since the introduction of continuous-time quantum walk algorithms that search on graphs [1], there is still no comprehensive theory as to which graphs support fast quantum search. Nevertheless, much work has been done to further our understanding. For example, we recently showed that global symmetry is unnecessary for fast quantum search [2].

Regarding specific graphs, a randomly walking quantum particle evolving by Schrödinger's equation searches on the complete graph, strongly regular graphs, and the hypercube in optimal $\Theta(\sqrt{N})$ time, the first of which is precisely the continuous-time analogue of Grover's algorithm [1–4]. Examples of these graphs are shown in Fig. 1. Additionally, such a particle can search on d-dimensional cubic lattices in $\Theta(\sqrt{N})$ total time when $d \geq 5$, and with progressively slower runtimes as d decreases [1,5,6], as shown in Table I.

One might suspect that fast search occurs when graphs are highly connected, as suggested by [1]. In this Letter, however, we show this intuition to be false by giving two examples of graphs for which the opposite holds true: one with low connectivity but fast search, and one with high connectivity but slow search; they are shown in Figs. 2 and 3, respectively. To do this, we first introduce four different ways to measure graph connectivity. Then we detail how a randomly walking quantum particle searches on a graph. Finally, we determine the runtimes of our two examples.

Measures of connectivity.—The two most common ways to measure connectivity are vertex connectivity and edge connectivity, which are how many vertices or edges must be removed to make a graph disconnected. For example, Fig. 2 has vertex and edge connectivities of 1 because removing the yellow or green vertex disconnects the graph, and so does removing the edge between them. Note that vertex connectivity is upper bounded by the edge connectivity, and both are upper bounded by the minimum degree of the graph. For the graphs in this Letter, the vertex and edge connectivities are equal.

Connectivity can also be measured using eigenvalues. The algebraic connectivity of a graph is the second-smallest eigenvalue λ_1 of its graph Laplacian L=D-A, where $D_{jj}=\deg(j)$ is a diagonal matrix with the degree of each vertex, and $A_{ij}=1$ if i and j are adjacent and 0 otherwise is the adjacency matrix [7]. Chosen this way, L is positive semidefinite. Its smallest eigenvalue λ_0 is 0, and it corresponds to the equilibrium state of diffusion. Since our graphs are connected, λ_1 is positive and quantifies how well diffusion occurs on the graph.

This can be improved by dividing L_{ij} by $\sqrt{\deg(i) \deg(j)}$ so that the diagonal terms become 1 and the off-diagonal

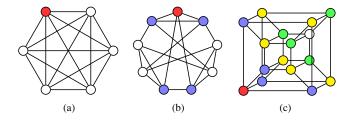


FIG. 1 (color online). (a) The complete graph with 6 vertices. (b) A strongly regular graph (Paley graph) with parameters (9, 4, 1, 2). (c) The four-dimensional hypercube. Without loss of generality, a marked vertex is colored red, and identically evolving vertices are identically colored.

TABLE I. Scalings of single runtimes and success probabilities for search on d-dimensional cubic lattices by quantum random walk, and the total runtimes with classical repetitions.

\overline{d}	Single runtime	Success probability	Total runtime
≥ 5	$N^{1/2}$	1	$N^{1/2}$
4	$\sqrt{N \log N}$	$1/\log N$	$\sqrt{N} \log^{3/2} N$
3	$N^{2/3}$	$1/N^{1/3}$	N
2	$N/\log N$	$(\log^2 N)/N$	$N^2/\log^3 N$

terms become $-1/\sqrt{\deg(i)\deg(j)}$ when i and j are adjacent and 0 otherwise. The eigenvalues of this "normalized" Laplacian $\mathcal L$ are no longer dependent on the number of vertices, and we take the second-smallest eigenvalue to be the normalized algebraic connectivity [8]. Note if the graph is k-regular, then the normalized Laplacian is related to the adjacency matrix and standard Laplacian by $\mathcal L = I - A/k = L/k$.

For the graphs we have introduced, all four of these connectivities are shown in Table II; see [9] for their references and derivations. With these in place, let us introduce the quantum search model and then find the runtimes of the examples (Figs. 2 and 3), showing they are faster or slower, respectively, than their connectivities might otherwise lead us to believe.

Quantum search on graphs.—The vertices of the graph correspond to computational basis states $\{|0\rangle,|1\rangle,...,|N-1\rangle\}$ of an N-dimensional Hilbert space. The system $|\psi(t)\rangle$ begins in an equal superposition of all the vertices $|s\rangle = \sum_{i=0}^{N-1} |i\rangle/\sqrt{N}$. Then it evolves by Schrödinger's equation with Hamiltonian $H = \gamma L - |a\rangle\langle a|$, where γ is the jumping rate (i.e., amplitude per time), L = D - A is the graph Laplacian, and $|a\rangle$ is the "marked" vertex we are searching for (i.e., the red vertex in Figs. 1, 2, and 3). For a k-regular graph, D = kI, so we can drop it by rezeroing the energy. Then the search Hamiltonian is

$$H = -\gamma A - |a\rangle\langle a|. \tag{1}$$

On the complete graph (i.e., Grover's problem), the system evolves in a two-dimensional subspace, and the squared overlaps of $|s\rangle$ and $|a\rangle$ with the eigenstates $|\psi_{0,1}\rangle$ of H are shown in Fig. 4. When γ is away from its critical value of $\gamma_c = 1/N$, then the initial equal superposition $|s\rangle$ is approximately $|\psi_0\rangle$ or $|\psi_1\rangle$ for large N, so the system approximately evolves only by phase multiplication. When $\gamma = \gamma_c$, however, the eigenstates are

$$|s\rangle \propto |\psi_0\rangle + |\psi_1\rangle |a\rangle \propto |\psi_0\rangle - |\psi_1\rangle,$$
 (2)

with an energy gap of $\Delta E = 2/\sqrt{N}$ [1]. Therefore the system evolves from $|s\rangle$ to $|a\rangle$ in time $\pi/\Delta E = \pi\sqrt{N}/2 = \Theta(\sqrt{N})$ [4]. This can also be proved using degenerate

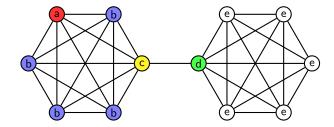


FIG. 2 (color online). A graph with 12 vertices constructed by joining two complete graphs of six vertices by a single edge.

perturbation theory [2], as we show rigorously for the next two examples in [1], but in this Letter we use the same graphical explanation as above.

Joined complete graphs.—For the first example, two complete graphs with N/2 vertices are joined by a single edge. We mark a vertex away from this "bridge" so that it is one of $N-2=\Theta(N)$ possible vertices, as opposed to one of two vertices on the bridge, which would be a trivial search problem. In Fig. 2, the marked vertex is colored red, and identically evolving vertices are the same color.

Intuitively, the bridge restricts probability from moving between the two complete graphs, so we are effectively searching on a single complete graph with N/2 vertices and total probability 1/2. Thus the success probability should reach 1/2 in time $\pi \sqrt{N/2}/2$, which is a total runtime of $\Theta(\sqrt{N})$ with the expected constant number of repetitions to boost the success probability near 1. This is the same optimal runtime as the highly connected complete graph, strongly regular graphs, and hypercube, even though the vertex or edge and normalized algebraic connectivities suggest it should be slower. Note this example does not discredit algebraic connectivity since the hypercube is also $\Theta(1)$, but the second example will.

To prove this intuition, note from Fig. 2 that the system evolves in a five-dimensional subspace, independent of N. Grouping identically evolving vertices, we get an orthonormal basis for this subspace,

$$|a\rangle = |\text{red}\rangle$$

$$|b\rangle = \frac{1}{\sqrt{N/2 - 2}} \sum_{i \in \text{blue}} |i\rangle$$

$$|c\rangle = |\text{yellow}\rangle$$

$$|d\rangle = |\text{green}\rangle$$

$$|e\rangle = \frac{1}{\sqrt{N/2 - 1}} \sum_{i \in \text{white}} |i\rangle.$$

Most of the vertices have degree N/2-1, except for the yellow and green vertices, which have degree N/2; for large N, however, they are asymptotically the same. Therefore, we assume that the graph is approximately regular. Then the search Hamiltonian (1) for large N is

TABLE II. The degrees and vertex, edge, algebraic, and normalized algebraic connectivities of various (nearly) regular graphs with N vertices.

Graph	Degree	Vertex or edge	Algebraic	Normalized algebraic
Complete	N-1	N-1	N	$N/(N-1) = \Theta(1)$
Strongly regular (type 1)	(N-1)/2	(N-1)/2	$(N-\sqrt{N})/2$	$(N - \sqrt{N})/(N - 1) = \Theta(1)$
Strongly regular (Latin square)	$d(\sqrt{N}-1)$	$d(\sqrt{N}-1)$	$(d-1)\sqrt{N}$	$(d-1)\sqrt{N}/[d(\sqrt{N}-1)] = \Theta(1)$
Hypercube	$\log_2 N$	$\log_2 N$	2	$2/\log_2 N = \Theta(1/\log N)$
d-dimensional cubic	2d	2d	$\approx 4\pi^2/N^{2/d}$	$\approx 2\pi^2/dN^{2/d} = \Theta(1/N^{2/d})$
Joined complete	$\approx N/2$	1	$\Theta(1)$	$\Theta(1/N)$
Simplex complete	$M = \Theta(\sqrt{N})$	$M = \Theta(\sqrt{N})$	1	$1/M = \Theta(1/\sqrt{N})$

$$H = -\gamma \begin{pmatrix} 1/\gamma & \sqrt{N/2 - 2} & 1 & 0 & 0\\ \sqrt{N/2 - 2} & N/2 - 3 & \sqrt{N/2 - 2} & 0 & 0\\ 1 & \sqrt{N/2 - 2} & 0 & 1 & 0\\ 0 & 0 & 1 & 0 & \sqrt{N/2 - 1}\\ 0 & 0 & 0 & \sqrt{N/2 - 1} & N/2 - 2 \end{pmatrix},$$

where the second item in the first row, for example, is from the adjacency matrix, and it is $1/\sqrt{N/2} - 2$ to convert between the normalizations of $|a\rangle$ and $|b\rangle$ times the N/2 - 2 blue vertices that connect to the red vertex.

Figure 5 shows the squared overlaps of $|s\rangle$ and $|a\rangle$ with the eigenstates of H. For large N, γ takes its critical value of $\gamma_c = 1/(N/2)$, at which half of $|s\rangle$ is proportional to $|\psi_0\rangle + |\psi_2\rangle$ (with the other half in $|\psi_1\rangle$) and $|a\rangle \propto |\psi_0\rangle - |\psi_2\rangle$ with an energy gap of $E_2 - E_0 = 2/\sqrt{N/2}$ [1]. Comparing this to (2), this is the same as searching on a complete graph with N/2 vertices and total probability 1/2,

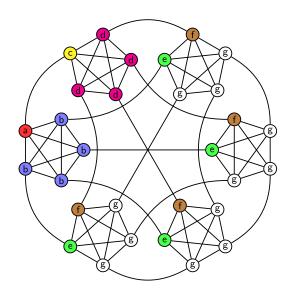


FIG. 3 (color online). A five-simplex with each vertex replaced with a complete graph of five vertices.

which proves that the success probability reaches 1/2 in time $\pi\sqrt{N/2}/2$. This can be seen in Fig. 6.

Simplex of complete graphs.—For the second example, we replace each of the M+1 vertices of an M-simplex with a complete graph of M vertices. An example with M=5 is shown in Fig. 3; the marked vertex is colored red, and identically evolving vertices are the same color. Note the vertices are homogeneous (i.e., the graph is vertex transitive), and there are N=M(M+1) total vertices. More formally, this is a first-order truncated M-simplex lattice, which has been studied in various statistical mechanics models [14,15]; the infinite-order recursive construction has also been studied using classical random walks [16].

From Fig. 3, the system evolves in a seven-dimensional subspace, independent of M. Grouping identically evolving vertices, we get an orthonormal basis for this subspace,

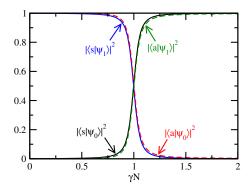


FIG. 4 (color online). Squared overlaps of $|s\rangle$ and $|a\rangle$ with eigenstates of H for search on the complete graph with N=1024.

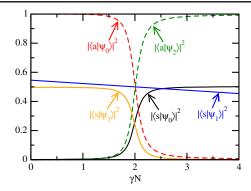


FIG. 5 (color online). Squared overlaps of $|s\rangle$ and $|a\rangle$ with eigenstates of H for search on joined complete graphs with 1024 total vertices.

$$\begin{split} |a\rangle &= |\text{red}\rangle \\ |b\rangle &= \frac{1}{\sqrt{M-1}} \sum_{i \in \text{blue}} |i\rangle \\ |c\rangle &= |\text{yellow}\rangle \\ |d\rangle &= \frac{1}{\sqrt{M-1}} \sum_{i \in \text{magenta}} |i\rangle \\ |e\rangle &= \frac{1}{\sqrt{M-1}} \sum_{i \in \text{green}} |i\rangle \\ |f\rangle &= \frac{1}{\sqrt{M-1}} \sum_{i \in \text{brown}} |i\rangle \\ |g\rangle &= \frac{1}{\sqrt{(M-1)(M-2)}} \sum_{i \in \text{white}} |i\rangle. \end{split}$$

Then the Hamiltonian (1) in this subspace is

$$H = -\gamma \begin{pmatrix} 1/\gamma & \sqrt{M_1} & 1 & 0 & 0 & 0 & 0 \\ \sqrt{M_1} & M_2 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & \sqrt{M_1} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{M_1} & M_2 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & \sqrt{M_2} \\ 0 & 0 & 0 & 1 & 1 & 0 & \sqrt{M_2} \\ 0 & 0 & 0 & 0 & \sqrt{M_2} & \sqrt{M_2} & M_2 \end{pmatrix},$$

where $M_1 = M - 1$ and $M_2 = M - 2$. The last item in the sixth row, for example, is from the adjacency matrix, and it is $\sqrt{M-1}/\sqrt{(M-1)(M-2)}$ to convert between the normalizations of $|g\rangle$ and $|f\rangle$ times the M-2 white vertices that connect to a brown vertex.

Figure 7 shows the squared overlaps of $|s\rangle$, $|a\rangle$, and $|b\rangle$ with the eigenstates of H, and it reveals a novel two-stage algorithm. First, we let γ equal $\gamma_{c1} = 2/M$, which is 0.02 in Fig. 7, because away from this critical value, the initial equal superposition $|s\rangle$ would approximately be an

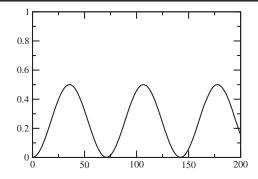


FIG. 6. Success probability as a function of time for search on joined complete graphs with 1024 total vertices.

eigenstate of H for large N, and then the system would approximately evolve only by phase multiplication. At this critical γ , roughly $|s\rangle \propto |\psi_0\rangle + |\psi_1\rangle$ and $|b\rangle \propto |\psi_0\rangle - |\psi_1\rangle$ with an energy gap of $4/M^{3/2}$ [1]. Comparing this with (2), the system evolves from $|s\rangle$ to $|b\rangle$ in time $\pi M^{3/2}/4$, as shown in Fig. 8.

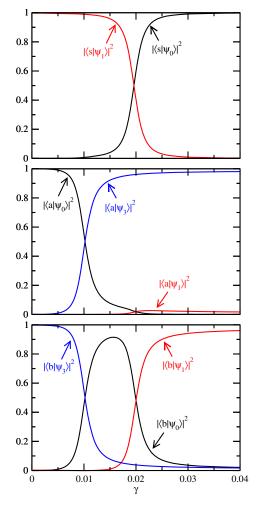


FIG. 7 (color online). Squared overlaps of $|s\rangle$, $|a\rangle$, and $|b\rangle$ with eigenstates of H for search on a simplex of complete graphs with M=100.

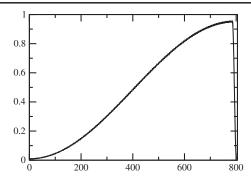


FIG. 8. Probability at $|b\rangle$ as a function of time for search on a simplex of complete graphs with M=100. Probability accumulates during the first stage of the algorithm from t=0 to $\pi 100^{3/2}/4 \approx 785.40$, and then it quickly leaves during the second stage, which takes $\pi \sqrt{100}/2 \approx 15.71$ time.

Now we change γ so it equals $\gamma_{c2}=1/M$, which is 0.01 in Fig. 7. While changing γ continuously appears in our nonlinear (quantum) search algorithms [17,18], such a discrete change is new. Then roughly $|b\rangle \propto |\psi_0\rangle + |\psi_3\rangle$ and $|a\rangle \propto |\psi_0\rangle - |\psi_3\rangle$ with an energy gap of $E_3 - E_0 = 2/\sqrt{M}$ [1]. Comparing this with (2), probability moves from $|b\rangle$ to $|a\rangle$ in time $\pi\sqrt{M}/2$, as shown in Figs. 8 and 9 with M=100, where the sudden dip and spike occurs when switching from the first to the second stage of the algorithm at $\pi 100^{3/2}/4 \approx 785.40$.

Together, the total runtime of this two-stage algorithm is $\pi M^{3/2}/4 + \pi \sqrt{M}/2 = \Theta(N^{3/4})$, which is slower than the $\Theta(\sqrt{N})$, $\Theta(\sqrt{N})$, and $\Theta(\sqrt{N}\log^{3/2}N)$ runtimes that vertex or edge, algebraic, and normalized algebraic connectivites would suggest by comparison to the (strongly regular) Latin square graph, hypercube, and four-dimensional cubic lattice, respectively.

These examples demonstrate that there is not a tight relationship between any of these measures of connectivity and the runtime of quantum random walk search algorithms, disproving the intuition that quantum search is fast as a consequence of high connectivity.

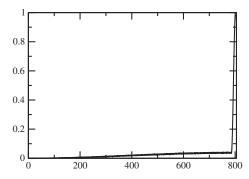


FIG. 9. Probability at $|a\rangle$ (i.e., the success probability) as a function of time for search on a simplex of complete graphs with M=100. During the second stage of the algorithm starting at $t=\pi 100^{3/2}/4\approx 785.40$ for a time of $\pi \sqrt{100}/2\approx 15.75$, the probability quickly accumulates.

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