An example of the difference between quantum and classical random walks

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In this note, we discuss a general definition of quantum random walks on graphs and illustrate with a simple graph the possibility of very different behavior between a classical random walk and its quantum analogue. In this graph, propagation between a particular pair of nodes is exponentially faster in the quantum case.

Introduction. Many classical algorithms are based on random walks, so it is natural to ask whether quantum random walks might be useful for quantum computation. A framework for using quantum random walks to solve decision problems was investigated in [1]. There also, an exponential separation was found between the classical and quantum times to propagate through a certain tree.

In this note, we describe a general definition of continuous-time random walks on graphs and give a simpler example of a graph for which the quantum time to propagate between a particular pair of nodes is exponentially shorter than the analogous classical propagation time. We also discuss advantages of the continuous time formulation over discrete versions.

Random walks. A continuous time classical random walk on a graph is a Markov process. A graph is a set of vertices \( \{1, 2, \ldots, v \} \) and a set of edges that specifies which pairs of vertices are connected in the graph. A step in a classical random walk on a graph only occurs between two vertices connected by an edge. Let \( \gamma \) denote the jumping rate. Starting at any vertex, the probability of jumping to any connected vertex in a time \( \epsilon \) is \( \gamma \epsilon \) (in the limit \( \epsilon \rightarrow 0 \)). This random walk can be described by the \( v \times v \) infinitesimal generator matrix \( M \) defined by

\[
M_{ab} = \begin{cases} 
-\gamma & a \neq b, \text{a and } b \text{ connected by an edge} \\
0 & a \neq b, \text{a and } b \text{ not connected} \\
\gamma & a = b, k \text{ is the valence of vertex } a.
\end{cases}
\]

If \( p_a(t) \) denotes the probability of being at vertex \( a \) at time \( t \), then

\[
\frac{dp_a(t)}{dt} = -\sum_b M_{ab} p_b(t).
\]

Consider quantum evolution in a \( v \)-dimensional Hilbert space according to a Hamiltonian \( H \). In a basis \( \{|1\}, |2\}, \ldots, |v\rangle \), the Schrödinger equation for \( |\psi(t)\rangle \) can be written

\[
i\hbar \frac{d}{dt}|\psi(t)\rangle = \sum_b (a|H|b\rangle \langle b|\psi(t)\rangle).
\]

Note the similarity between (2) and (3). Whereas (2) conserves probability in the sense that

\[
\sum_a p_a(t) = 1,
\]

the Schrödinger equation preserves probability as the sum of the amplitudes squared:

\[
\sum_a |\langle a|\psi(t)\rangle|^2 = 1.
\]

In some sense, any evolution in a finite-dimensional Hilbert space can be thought of as a “quantum random walk.” However, the analogy is clearest when \( H \) has an obvious local structure.

A quantum random walk on a graph is naturally defined in a Hilbert space spanned by basis elements corresponding to the vertices. To respect the structure of the graph, we require that for \( a \neq b \),

\[
\langle a|H|b\rangle \neq 0 \text{ iff } a \text{ and } b \text{ are connected by an edge}.
\]

This is a very weak requirement, so we can impose more structure on \( H \). A natural quantum analogue to the classical random walk described above is given by the Hamiltonian with matrix elements (7)

\[
(a|H|b) = M_{ab}.
\]

Note that on a one-dimensional lattice, this results in the Hamiltonian defined by

\[
H|j\rangle = -\frac{1}{\Delta^2}(|j-1\rangle - 2|j\rangle + |j+1\rangle),
\]

which is just a discrete approximation to the operator \(-d^2/dx^2 \) (where \( \Delta = \gamma^{-1/2} \) is the lattice spacing).

The difference between the quantum and classical evolution comes from the \( i \) which appears in (3) but not in (2). This can result in radically different behavior, as seen in (4). A simpler example is given next.

An example. Here we define a sequence of graphs \( G_n \). The number of vertices in \( G_n \) is \( 2^{n+1} + 2^n - 2 \). In Figure 1, we show \( G_4 \). In general, \( G_n \) consists of two balanced binary trees of depth \( n \) with the \( 2^n \) \( n \)-th-level vertices of the two trees pairwise identified.
vertices in column $j$, that is,

$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column } j} |a\rangle,$$

(9)

where

$$N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n-j} & n \leq j \leq 2n. \end{cases}$$

(10)

In this basis, the non-zero matrix elements of $H$ are

$$\langle \text{col } j|H|\text{col } j \pm 1\rangle = -\sqrt{2}\gamma$$

(11)

$$\langle \text{col } j|H|\text{col } j\rangle = \begin{cases} 2\gamma & j = 0, n, 2n \\ 3\gamma & \text{otherwise}, \end{cases}$$

(12)

which is depicted in Figure 2 (for $n = 4$) as a quantum random walk on a line with $2n+1$ vertices.

Starting at the leftmost vertex of Figure 2, there is an appreciable probability of being at the rightmost vertex after a time proportional to $n$. To see this, first consider quantum propagation on an infinite, translationally invariant line of vertices as depicted in Figure 3. Here it is straightforward to compute the amplitude to go from vertex $l$ to vertex $m$ in a time $t$ (for example, see [3]):

$$\langle m|e^{-iHt}|l\rangle = e^{-i3\gamma t}i^{m-l}J_{m-l}(2\sqrt{2}\gamma t),$$

(13)

where $J_{m-l}$ is a Bessel function of order $m-l$. This corresponds to propagation with speed $2\sqrt{2}\gamma$. More precisely, for any $\epsilon > 0$ and $|m-l| \gg 1$, for $t < \left(\frac{1}{2\sqrt{2}\gamma} - \epsilon\right)|m-l|$, the amplitude is exponentially small in $|m-l|$, whereas there are values of $t$ between $\left(\frac{1}{2\sqrt{2}\gamma}\right)|m-l|$ and $\left(\frac{1}{2\sqrt{2}\gamma} + \epsilon\right)|m-l|$ at which the amplitude is of order $|m-l|^{-1/2}$.

In the limit of large $n$, the reduced version of $G_n$ is nearly identical to the infinite, translationally invariant line, so it is plausible that propagation on $G_n$ will also occur with speed $2\sqrt{2}\gamma$. To verify this, we numerically compute the probability $|\langle \text{col } j|\psi(t)\rangle|^2$ of being in column $j$ at various times $t$, where $|\psi(0)\rangle = |\text{col } 0\rangle$ and we choose $\gamma = 1$. This is shown in Figure 4 with $n = 500$ for
$t = 100, 250, \text{ and } 400$. These plots clearly show a wave packet which propagates with speed $2\sqrt{2}$, with the amplitude near the wavefront decreasing like $t^{-1/2}$. In the first plot, at $t = 100$, the leading edge of the distribution is at column $200\sqrt{2} \approx 283$. The packet has not yet encountered the small defect at the center, so it has a relatively simple shape. At $t = 250$, the wavefront has passed the center, and a small reflection can be seen propagating backward. However, the leading edge is relatively undisturbed, having propagated to column $500\sqrt{2} \approx 707$. The wavefront continues to propagate with speed $2\sqrt{2}$ until it reaches the right root, where the packet is reflected. The last plot, at $t = 400$, shows the distribution shortly after this first reflection. Even after the reflection, there is still an appreciable probability of being at the right root.

The limiting distribution. In this section, we consider the distribution over the vertices after a long time. We emphasize that although the mixing times (the characteristic times to reach the limiting distribution) may be similar in the classical and quantum cases [3], this is in no way indicative of similar dynamics, as the limiting distributions may be radically different.

In the classical case, the limiting distribution is defined as

$$\pi_b = \lim_{T \to \infty} p_b(T),$$  \hspace{1cm} (14)

which is independent of the starting state. It is easy to see that the limiting distribution on $G_n$ is uniform over the vertices: this distribution is the unique eigenvector of $M$ with eigenvalue 0, so it is the only component that remains after a long time. Thus $\pi_b = (2^{n+1} + 2^n - 2)^{-1}$ for each vertex $b$, which is exponentially small.

In the quantum case, unitarity prevents the walk from reaching a steady state. However, a sensible definition of the limiting distribution, which depends on the initial state $|a\rangle$, is given by

$$\chi_b = \lim_{T \to \infty} \frac{1}{T} \int_0^T |\langle b | e^{-iHt} | a \rangle|^2 \, dt.$$ \hspace{1cm} (15)

This is the distribution resulting from a measurement done after a time chosen uniformly in $[0, T]$, in the limit of large $T$. By expanding over the energy eigenstates $|E_r\rangle$, we find

$$\chi_b = \sum_{r,s} \langle b | E_r \rangle \langle E_r | a \rangle \langle a | E_s \rangle \langle E_s | b \rangle \times \lim_{T \to \infty} \frac{1}{T} \int_0^T e^{-i(E_r - E_s)t} \, dt$$

$$= \sum_r \langle a | E_r \rangle^2 \langle b | E_r \rangle^2$$ \hspace{1cm} (16) (note that we have assumed $E_r \neq E_s$ for $r \neq s$, which is true for $G_n$). In particular, consider the case where $|a\rangle = |\text{col } 0\rangle$ corresponds to the left root and $|b\rangle = |\text{col } 2n\rangle$ corresponds to the right root. In this case, we may work in the reduced Hilbert space spanned by the columns, so the number of energy eigenstates is $2n + 1$. By symmetry, $|\langle \text{col } 0 | E_r \rangle| = |\langle \text{col } 2n | E_r \rangle|$. The Cauchy-Schwartz inequality gives

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{Propagation in $G_{500}$ starting at the left root. From top to bottom, the times are $t = 100, 250, \text{ and } 400$.}
\end{figure}
\[
\sum_r |\langle \text{col 0}|E_r \rangle|^4 \leq \left( \sum_r |\langle \text{col 0}|E_r \rangle|^2 \right)^2 = 1, \tag{18}
\]
which implies
\[
\sum_r |\langle \text{col 0}|E_r \rangle|^4 \geq \frac{1}{2n+1}. \tag{19}
\]
Thus in the limiting distribution, the probability of being at the right root, starting at the left root, is
\[
\chi_{\text{col 2n}} \geq \frac{1}{2n+1}, \tag{20}
\]
which is much larger than in the classical case.

**Discussion.** The model of quantum random walks used in this note applies automatically to any graph. In particular, the Hamiltonian is determined by the local structure of the graph and its definition does not require knowledge of any global properties. It is easy to imagine situations where the local structure of a graph is readily accessible, but determining some global property is difficult. For example, a computational problem may involve searching a graph for a node with a certain property whose presence or absence from the graph corresponds to the solution of an NP-complete problem [1].

The Hamiltonian-based approach to quantum random walks can be contrasted with discrete time models (for example, see [3–5]) involving the extra state space of a “quantum coin.” This extra label seems to be necessary in discrete time formulations of quantum random walks (and is provably necessary in the one dimensional case [6]). However, for general graphs of mixed valence, it is not obvious how to define the discrete time unitary evolution operator without knowledge of global properties of the graph.

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