What Quantum Walks can do that Classical ones can not.

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Classical Random Walks

• Stationary, ergodic and irreversible.

• Discrete and continuous time. Properties linked to Laplacian matrix, and in continuous time case determined by heat kernel.

• Lead to a variety of graph-based algorithms for problems such as routing, information retrieval and shape analysis.
Quantum walks

- Non-stationary, non-ergodic and reversible,

- Discrete and continuous time versions. Discrete time based on Hadamard coin. Continuous time controlled by Schrödinger equation with Laplacian as Hamiltonian.

- Can hit exponentially faster than classical walk.
Continuous time walk

• Classical

\[ \frac{d}{dt} p(t) = -Lp(t) \]

• Quantum

\[ \frac{d}{dt} |\varphi_t\rangle = -iL |\varphi_t\rangle \]
Continuous time walk

- Classical (heat equation)
  \[
  \frac{d}{dt} p(t) = -Lp(t)
  \]
  \[
  p(t) = \exp[-Lt] p(0)
  \]

- Quantum (complex wave equation)
  \[
  \frac{d}{dt} |\varphi_t\rangle = -iL |\varphi_t\rangle
  \]
  \[
  |\varphi_t\rangle = \exp[-iL] |\varphi_0\rangle
  \]
Walks compared

Classical walk

Quantum walk
Quantum vs Classical

- Hitting time behavior of quantum walks is completely different from its classical counterpart (see Fig. quantum vs classical on a line)
Why interesting

- Classical walk characterised by probability state-vector.

- In quantum case characterised by a complex wave function.

- In quantum case interference and entanglement lead to interesting phenomenon, not present in classical case.
Relations to Symmetry

- Symmetrical substructures result in destructive and constructive interference patterns.
- Interference leads to cancellation of backtracking paths and faster hitting times.
Uses in ML/PR

• Interference effects endow QW algorithms with properties not exhibited by classical walks - quantum weirdness.

• Lift co-spectralities – better distinguish trees and strongly regular graphs – (Emms etc al PR 2009).

• Quantum commute time – shows long range symmetry sensitivity (Emms, QIC 2010).

• Quantum information theory of walk leads to symmetry detection (Rossi et al Phys Rev E, 2013) and new family of symmetry sensitive graph kernels.
Embedding using commute time
Hitting time

\( Q(u,v) \): Expected number of steps of a random walk before node \( v \) is visited commencing from node \( u \).
Commute time

$CT(u,v)$: Expected time taken for a random walk to travel from node $u$ to node $v$ and then return again

$CT(u,v) = Q(u,v) + Q(v,u)$
Idea: compute edge attribute that is robust to modifications in edge-structure.

Commute time: averages over all paths connecting a pair of nodes. Effects of edge deletion reduced.
Commute Time Embedding

- Commute time given by Laplacian spectrum

\[ CT(u, v) = \text{vol} \sum_{i=2}^{\left|V\right|} \frac{1}{\lambda_i} \left( \frac{\phi_i(u)}{\sqrt{d_u}} - \frac{\phi_i(v)}{\sqrt{d_v}} \right)^2 \]

- Embedding that preserves commute time has co-ordinate matrix (vectors of co-ordinates are columns):

\[ Y = \sqrt{\frac{\text{vol}}{\Lambda D}} \Phi^T \]
Example embedding

Fig. 1. Original planar graph.

(a) Normalised Laplacian Embedding.  (b) Commute Time Embedding.

Fig. 2. Graph embedding comparison.
CT embedding used to pose Costiera and Kanade multibody motion analysis as clustering problem.
Embeddings
Commute times of quantum walks
Hitting time

• Probability that walk is at node $v$ at time $t$

\[ P(X_u^t = v) = |\langle v | \exp[-iLt]u \rangle|^2 \]

• Cumulative probability density

\[ \frac{d}{dt} R(t) = P(X_u^t = v)[1 - R(t)] \]

• Hitting time

\[ O(u, v) = \int_0^\infty R(t)dt \]
Average commute vs path length

Quantum walk reduces effect of path length.

Quantum

Classical
Classical vs quantum commute time

Scatter plot of classical commute time against quantum commute time

Relationship is not deterministic
Symmetries

- Project nodes of graph into subspace spanned by eigenvectors of commute time matrix.
- Symmetrically positioned nodes project onto same point in subspace.
- Eigenvectors sort nodes according to symmetries.
- Effective commute time reduced between symmetrically placed nodes.
- Due to cancellation of interference amplitude,
- Accounts for speed up in hitting time.
Embeddings of cojoined trees: Classical and quantum commute times. In case of quantum commute time, symmetrically placed nodes embed to same location is subspace.
Embedding of a wheel with 4 spokes

Fig. 11. Quantum and classical hitting time embeddings of the 32 vertex ‘wheel’ with 4 ‘spokes’.
Fig. 12. Coincident vertices in the $d^{th}$ dimension of the quantum hitting time embedding of the 32 vertex 'wheel' with 4 'spokes'. Coincident vertices are labelled with the same colour and number.
Problems

• Commute time is not a quantum observable.

• Does not work with approximate symmetries.

• Need a more principled way of comparing quantum walks and their interferences.

• Use density matrices and quantum Jensen-Shannon divergence.
Quantum Mechanical Background

- Given a graph $G = (V,E)$, a continuous-time quantum walk is defined as a time evolving quantum state $|\psi_t\rangle \in \mathbb{C}^{|V|}$ over $V$.
- A quantum state is a complex linear combination of the basis states $|u\rangle$.

$$|\psi_t\rangle = \sum_{u \in V} \alpha_u(t) |u\rangle$$

- The probability of observing a quantum walker at node $u$ at time $t$ is

$$\Pr(X^t = u) = \alpha_u(t)\alpha_u^*(t)$$

$$\sum_{u \in V} \alpha_u(t)\alpha_u^*(t) = 1 \quad \alpha_u(t) \in \mathbb{C}$$
Density Operators

- A pure state is a state that can be described by a single ket vector.
- Consider a (probabilistic) ensemble of quantum states $|\psi_i\rangle$ with probability $p_i$.
- Define density operator of such ensemble as

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$

- Density operators model observation probabilities for ensemble states.
  - The probability of observing a quantum walker in a state $\varphi$

Quantum Jensen-Shannon Divergence

- The Von Neumann entropy of a density operator is

\[ H_N(\rho) = -Tr(\rho \log \rho) = - \sum_j \lambda_j \log \lambda_j \]

- The quantum Jensen-Shannon divergence between two density operators is

\[ D_{JS}(\rho, \sigma) = H_N\left(\frac{\rho + \sigma}{2}\right) - \frac{1}{2}H_N(\rho) - \frac{1}{2}H_N(\sigma) \]

- Generalization of classical Jensen-Shannon divergence to quantum states
  - Always well defined, symmetric, negative definite and bounded between 0 and 1
  - For pure states it is proved to be the square of a metric, for mixed states we only have empirical evidence suggesting it.
FIG. 3. A star graph with 4 nodes and a modified version where two leaves are connected by an extra edge representing structural noise. The bar graph shows that although the symmetry between nodes 2-3 and nodes 2-4 is broken with the addition of an extra edge, the QJSD is still sensibly higher for those pairs of nodes, suggesting the presence of an approximate symmetry.
FIG. 4. (Color online) The average QJSD as a function of the structural (edge) noise for a $5 \times 5$ grid and a complete graph. Adding by randomly deleting (inserting) edges has the effect of breaking the symmetries of the original graphs and as a consequence the average QJSD decreases. Here the solid line indicates the mean, while the dashed lines indicate the standard deviation.
Avg. QJSD vs Time

(a) 5 × 5 Grid

(b) Wheel

FIG. 5. (Color online) The average of the QJSD matrix clearly distinguishes between a random graph and a symmetrical graph where artificial noise is added. Here the solid line indicates the mean, while the dashed lines indicate the standard deviation.
Measuring Graph Similarity

• Can measure the degree of similarity between two graphs by merging them into a new superstructure which is maximally symmetric when the original graphs are isomorphic. QJSD gives us an information theoretic graph kernel.

• We define two walks on this composite structure such that their divergence is maximal when the two original graphs are isomorphic

\[
|\psi_t^+\rangle = \sum_{u \in V} \psi_{0u}^+ |u\rangle \\
\psi_{0u}^+ = \begin{cases} 
+\frac{d_u}{C} & \text{if } u \in G_1 \\
+\frac{d_u}{C} & \text{if } u \in G_2
\end{cases}
\]

\[
|\psi_t^-\rangle = \sum_{u \in V} \psi_{0u}^- |u\rangle \\
\psi_{0u}^- = \begin{cases} 
+\frac{d_u}{C} & \text{if } u \in G_1 \\
-\frac{d_u}{C} & \text{if } u \in G_2
\end{cases}
\]

**Fig. 1.** Given two graphs \(G_1(V_1, E_1, \nu_1)\) and \(G_2(V_2, E_2, \nu_2)\) we build a new graph \(G = (V, E)\) where \(V = V_1 \cup V_2, E = E_1 \cup E_2\) and we add a new edge \((u, v)\) between each pair of nodes \(u \in V_1\) and \(v \in V_2\).
Quantum walks interfere

• Allows us to define matrix representations of graphs (strongly regular graphs, trees) that can lift problems of co-spectrality (PR 2009).

• Representation found by constructing orientated line graph – and related to Ihara zeta function (QIP, 2011).

• Measure symmetries in graphs (QIC 2009, Phys. Rev E, 2013)

• Construct new families of graph-kernels that respond to structure in a more global way, and can avoid backtracking (IEEE TNNLS 2013).