Analysis of Entropy in Random and Quantum Walks on Graphs

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Introduction

Random walks and Quantum walks are foundational paradigms in studying stochastic processes. While a random walk can be summed up as a series of random movements within a graph, a quantum random walk introduces the wave-like properties of quantum mechanics such as superposition and interference into this process. In fact, any quantum algorithm can be a mapped to a quantum walk on a graph.

Analyzing these walks has broad implications, from machine learning to medicine manufacturing. For instance, quantum walks may provide ways to speed-up the PageRank algorithm that drives web-page recommendation. In addition, they are candidates for the efficient simulation of quantum systems, a problem considered to be intractable for classical computers.

Background

Qubits: State represented as vector in bi-dimensional Hilbert space. Unlike bits, qubits are in an undefined superpositions of states 0 and 1 until a measurement is performed.

Graphs: mathematical structures composed of nodes and edges representing the relationship between pairs of objects.

Quantum Gates: Unitary operations on the Hilbert space spanned by qubits. Transform the state preserving norm.

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix} \quad \boxed{H}$$

Fig 1: Hadamard gate

$$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}$$

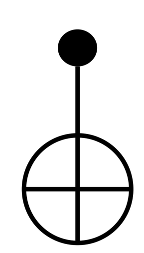


Fig 2: CNOT gate

Quantum Circuits: Sequence of quantum gates that manipulates qubits to perform a quantum algorithm. Serve as a universal quantum computing model.

Random Walk: Stochastic process on vertices of a graph. Position is a random variable.

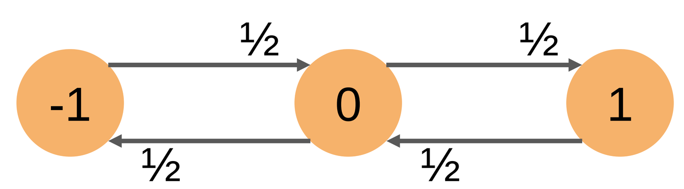


Fig 3: Random walk on path graph.

Quantum Walk: evolution of superposition of graph edges. Measurements generate probability distribution on vertices.

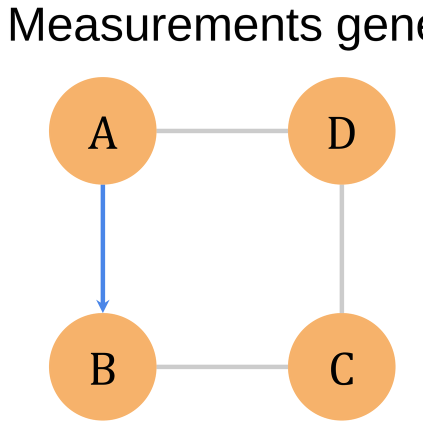


Fig 4: Initial state. $|\Psi(0)\rangle = |A, B\rangle$.

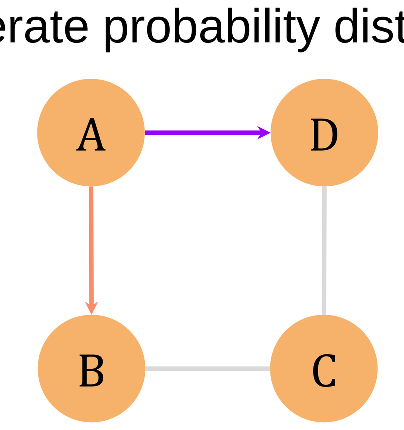


Fig 5: Coin yields $C|\Psi(0)\rangle$ as $\alpha|A, B\rangle + \beta|A, D\rangle$

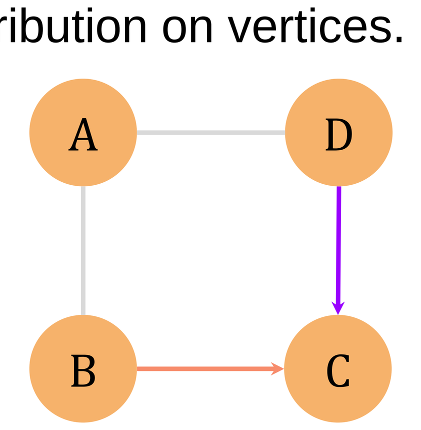


Fig 6: Shift yields $SC|\Psi(0)\rangle$ as $\alpha|B, C\rangle + \beta|D, C\rangle$

Contributions

We investigated entropy in walks on cycle and torus graphs to derive intuition on:

1. Comparison between random and quantum walks
2. Impact of initial conditions in evolution of entropy
3. Effects of real hardware noise in system's evolution

Experiments

Random walks

- Create walk matrix P from adjacency matrix
- Define initial probability distribution $\boldsymbol{\pi}(0)$
- Compute $\boldsymbol{\pi}(k) = P^k\boldsymbol{\pi}(0)$ for k = 1,2,..., t
- Compute entropy $H[\boldsymbol{\pi}(k)]$ for k = 1,2,..., t

$$\begin{bmatrix}0 & ½ & 0 & ½\\ ½ & 0 & ½ & 0\\ 0 & ½ & 0 & ½\\ ½ & 0 & ½ & 0\end{bmatrix}$$

Fig 7: 4-node cycle random walk transition matrix

$$\boldsymbol{\pi}(k+1) = P\boldsymbol{\pi}(k)$$

Eq 1: Random walk

$$|\Psi(k+1)\rangle = SC|\Psi(k)\rangle$$

Eq 2: Quantum Walk

$$H[\boldsymbol{\pi}(k)] = -\Sigma_x \boldsymbol{\pi}_x(k)\log[\boldsymbol{\pi}_x(k)]$$

Eq 3: Vertex probability distribution entropy

Quantum walks

- Define coin (C) and shift (S) operators using Qiskit
  - Hadamard gate used as coin to compare with uniform random walk
- Initialize initial state $|\Psi(0)\rangle$ of the walker
- Perform circuit $|\Psi(k)\rangle = (SC)^k|\Psi(0)\rangle$ for k = 1,2,..., t
  - Repeat and measure system to estimate $\boldsymbol{\pi}(k)$
- Calculate the entropy $H[\boldsymbol{\pi}(k)]$ for k = 1,2,..., t

Coin	Input	Output
0	00	11
0	01	00
0	10	01
0	11	10
1	00	01
1	01	10
1	10	11
1	11	00

Fig 8: Truth table for a 4-node cycle quantum walker position.

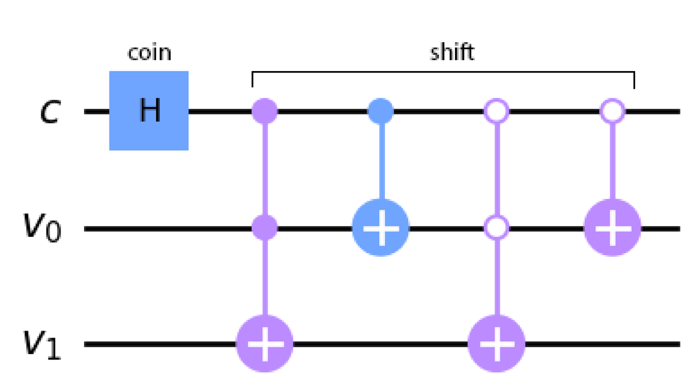


Fig 9: Quantum circuit for a 4-node cycle QWalk

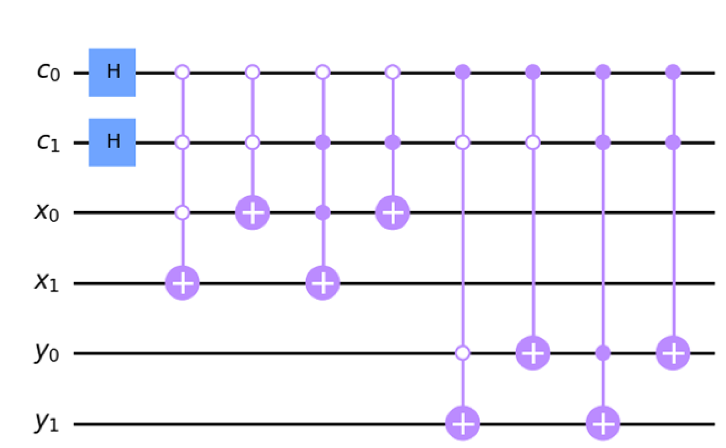
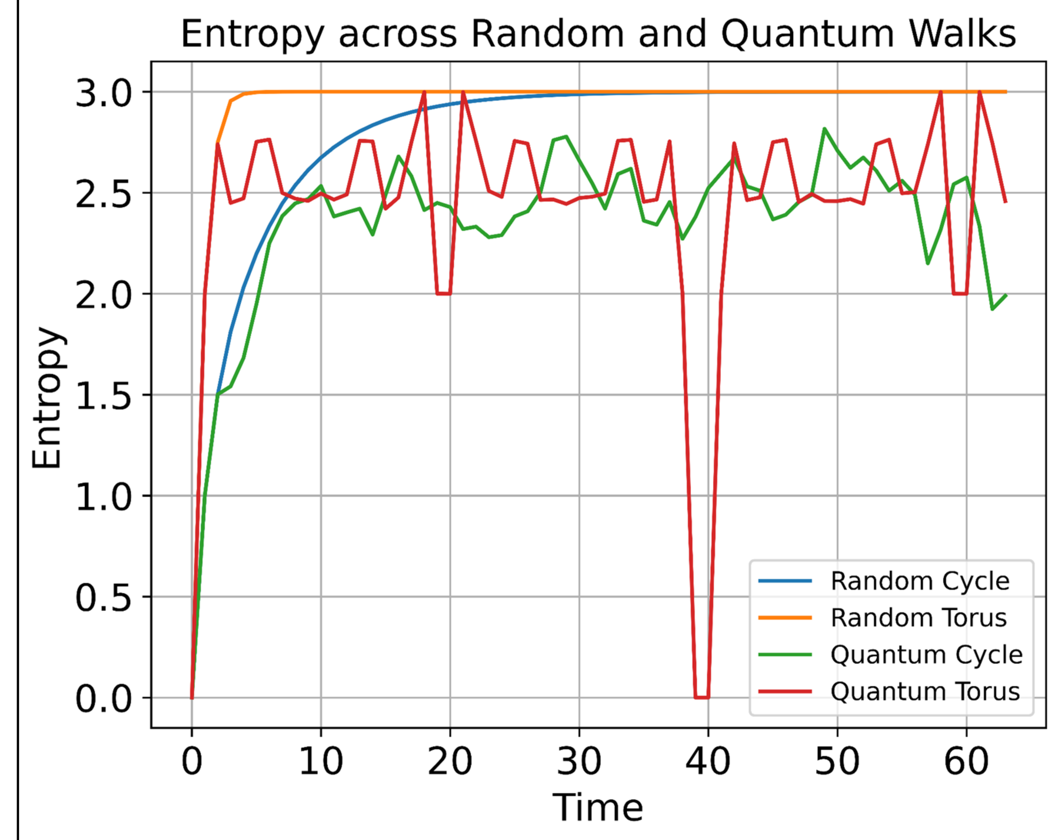


Fig 10: Quantum circuit for a 4x4-node torus quantum walk

Results and Discussion

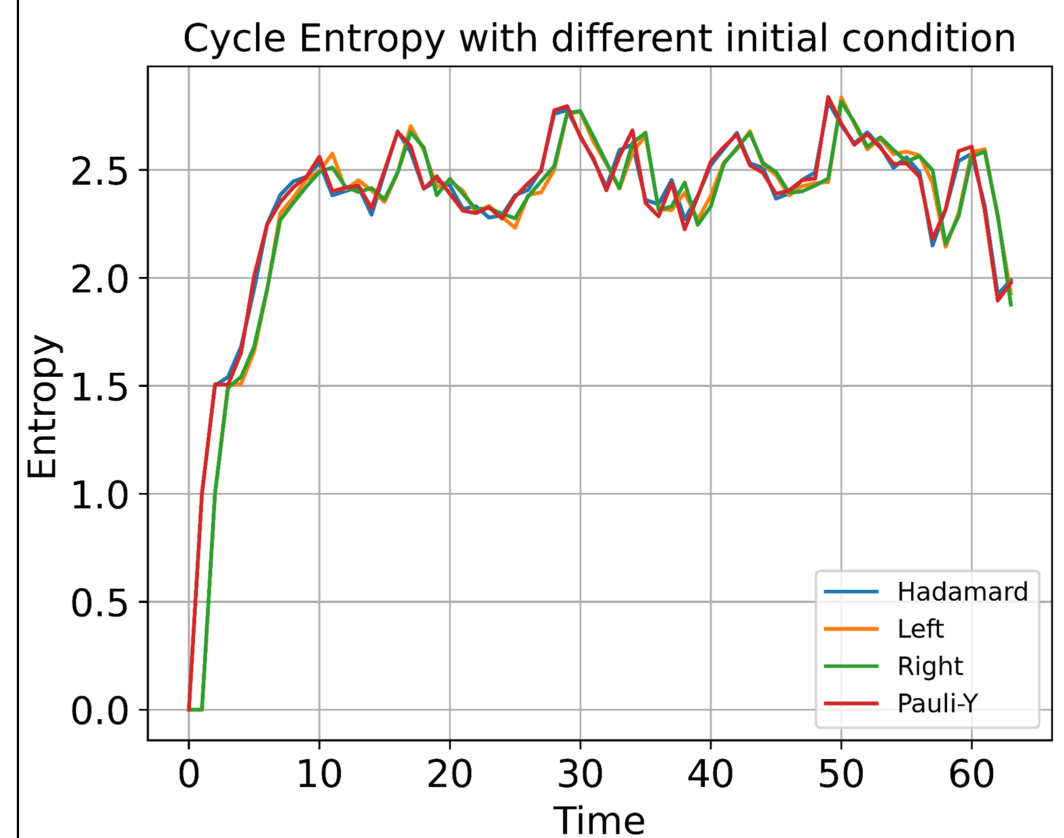


Random walks

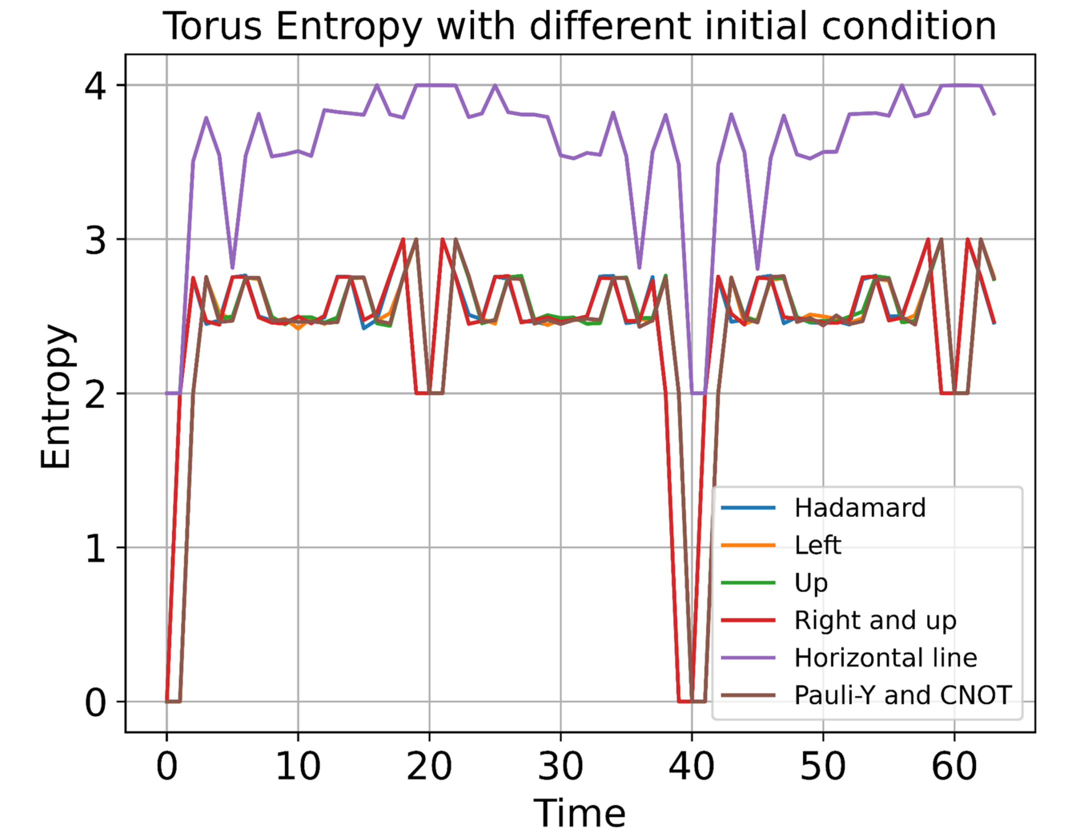
- Vertex probabilities converge
- Entropy strictly increases for random walks
- Entropy on torus grows faster than cycle
- Growth rate explained by mixing times

Quantum Walks

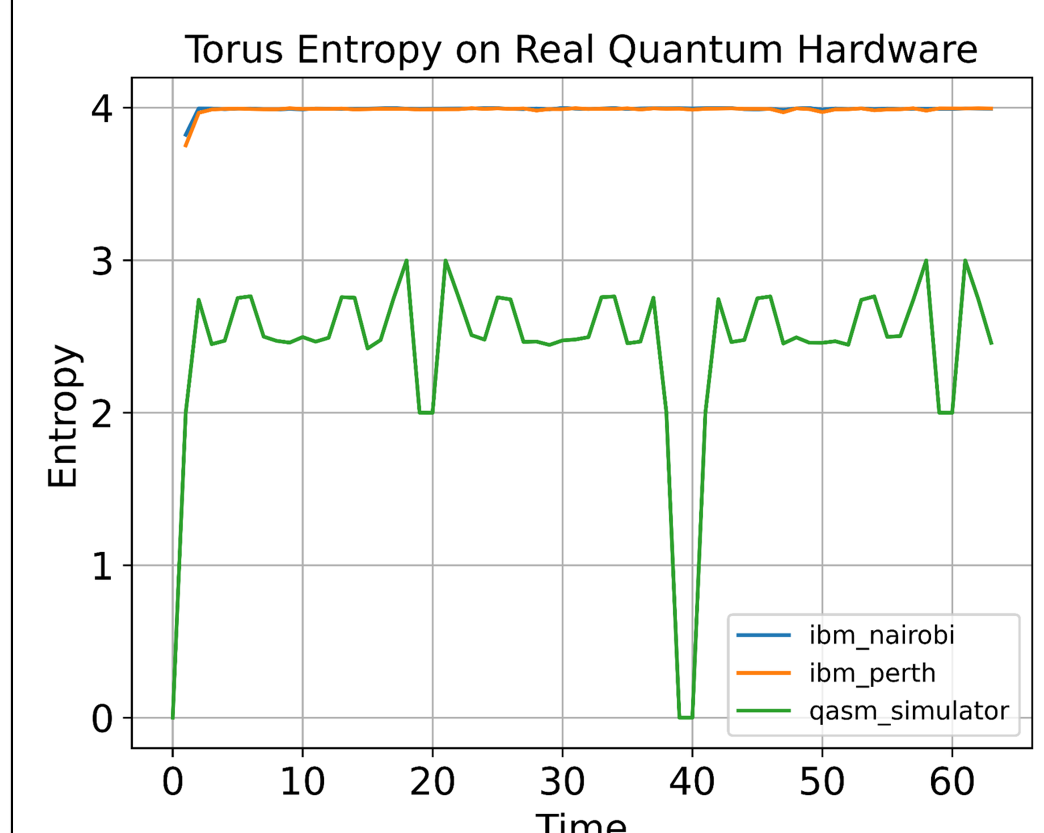
- Vertex probabilities don't converge
- Seem to "defy" second law of thermodynamics
- Entropy fluctuates over time, dropping to zero once.



- Entropy behaves similarly for cycle with different initial coin conditions cycle
- Indicates a non-trivial dependence between entropy and initial state



- Lowest four curves follow similar pattern
- Horizontal line initial condition causes different dynamics
- Similar oscillatory behavior for all five curves, (including dip point around t = 40)
- Indicates that initial entropy plays important role



- Stark divergence between simulation and experiments
- Current quantum computers inaccurate
- IBM's Nairobi and Perth show high entropies at all times (independent of circuit size).

Future work

- Extend analysis on impacts of initial condition on entropy
- Study quantum walks on more generic graphs
- Search for quantum walk operators that reduce initial entropy
- Analyze entropy oscillations theoretically