Characterizing the Relationship Between Unitary Quantum Walks and Non-Homogeneous Random Walks

Matheus Guedes de Andrade[1], **Franklin de Lima Marquezino**[1], **Daniel Ratton Figueiredo**[1]

[1]Programa de Engenharia de Sistemas e Computação (PESC)
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia (COPPE)
Universidade Federal do Rio de Janeiro (UFRJ)

1. Introduction

It is unquestionable that quantum computing has the power to disrupt science and technology, enabling new applications in different domains and extending the range of efficiently computable problems [Shor 1994, Lubasch et al. 2020]. Quantum computing is already a reality and different small scale quantum computers have been built by different corporations (such as the superconducting computers from Google or Rigetti, and the photonic computer from Xanadu) and some options are even available to the general public (as the IBM Q Experience). However, programming a quantum computer is drastically different from programming a classic computer, since the former relies directly on the quantum properties of matter to perform computations. Indeed, a drawback to quantum computing is the lack of a generic framework to guide the design of quantum algorithms.

A quantum walk is a model to encode a moving particle on a graph by considering the superposition of quantum states [Aharonov et al. 1993]. Although originally conceived as the quantum counterpart of the classic random walk, quantum walks are universal for quantum computing [Childs 2009], meaning that any quantum algorithm can be expressed as a quantum walk, and thus described as a moving quantum particle on a graph. This opens the possibility of using quantum walks as a generic framework to design quantum algorithms.

Similarly, random walks play a fundamental role in the development of various algorithms, like PageRank for ranking network nodes and other algorithms for searching, clustering and sampling network nodes. The success of random walks as a tool for building algorithms stems from its simplicity and predictability as a random model. Recall that a random walk is a model for a moving particle on a graph where at each time step the particle moves to an neighboring node chosen uniformly at random.

Since their inception, the connection between quantum and random walks has been investigated. Early results on quantum walks identified significant differences with respect to random walks, in particular that the wavefunction of quantum walks do not converge to a fixed superposition of states and that the node probability distribution does not necessarily converge [Portugal 2013]. Nonetheless, these differences were obtained under the assumption of time-homogeneous random walks and quantum walks with time-independent unitary operators. When these two assumptions are relaxed, the representation power of both random and quantum walks increases significantly, giving rise to much more powerful models.

Indeed, under the assumption that random walks are not time-homogeneous, recent prior work has shown that random walks can be constructed to be statistically equivalent to quantum walks on an infinite line graph [Montero 2017]. However, the potential of

non-homogeneous random walks is far greater and establishing a more general connection with quantum walks remained an open question.

1.1. Main challenges and goals

The goal of this thesis is to establish a broad and theoretical connection between random walks and quantum walks in a discrete time model. While recent works have explored this connection for specific scenarios, the aim here is to establish a more general result. In particular, the dynamics of the random walk and quantum walk should occur over the same underlying and arbitrary graph. Moreover, quantum walk evolution is not constrained to any specific operator and requires only to be unitary. Last, while prior works have investigated this equivalence for a single walker, the goal here is to also consider a scenario where the quantum system is formed by multiple quantum walkers interacting with one another. Can random walks match such dynamics? The challenge is to devise a theoretical framework where the equivalence can be rigorously established.

A general connection between the two walks also opens the possibility of simulating quantum walks through the simulation of random walks. Thus, a second goal of this thesis is to show that random walks can be used to simulate quantum walks. In particular, that the vertex probability yielded by the quantum system at an arbitrary time is reconstructed by simulating the random walk up to the same time instant. In this context, the fundamental challenge involved is an efficient algorithm for the construction of such random walk.

1.2. Results achieved

This thesis delivered on its goals making three main contributions:

- A theorem establishing that the vertex probability distribution over time of any unitary quantum walk on a finite graph can be represented by a time-dependent random walk. The proof is by construction and provides the procedure to build an statistically equivalent time-dependent random walk for every time step of the quantum walk. The result is extended to the case of multiple quantum walkers that can possibly interact with one another. This contribution has been published in a leading journal in Quantum Computing [Andrade et al. 2020].
- The second main contribution goes on the opposite direction of the first: a theorem establishing that the probability distribution over time of any random walk on a finite graph can be represented by a time-dependent quantum walk. Again, the proof is by construction and provides the procedure to build a unitary time-dependent quantum walk that is to be measured at the desired time instant. This contribution is currently under revision and pre-print is available [Andrade et al. 2021].
- A simulation procedure for quantum walks based on its equivalent time-dependent random walk. This procedure allows for the simulation of *quantum walk trajectories* a concept that essentially brings the idea of sample paths in random walks to quantum walks. The idea of quantum walk trajectories (and how to generate them) is also a contribution of this thesis. This contribution has been published in the same article as the first contribution [Andrade et al. 2020].

The remainder of this article is organized as follows. A minimal theoretical background and notation is provided in Section 2. In Section 3, the first and third contributions are described in detail. Section 4 presents the second contribution.

2. Background

Let $G = (V, E)$ be a symmetric directed graph. A discrete time random walk on G can be characterized by a time-dependent probability vector $\pi(t) : \mathbb{N} \to \mathbb{R}^{|V|}$ described by the matrix equation

$$\pi(t+1) = P(t)\pi(t), \tag{1}$$

where $\pi_v(t)$ denotes the probability that the walker is in vertex v at instant t, and $P(t)$ is a column-stochastic matrix with entries $p_{vu}(t)$ representing the transition probability for the walker to move from vertex u to v. Essentially, Equation 1 shows that the probability of a vertex v at instant $t+1$ is a combination of the probabilities of the neighbors of v at instant t, a property we refer to as the local evolution of probabilities.

A discrete-time coined quantum walk on G describes the evolution of a complex vector $|\Psi(t)\rangle \in \mathbb{C}^{|E|} = \mathcal{H}_w$, where the space $\mathcal{H}_w = \mathcal{H}_v \otimes \mathcal{H}_c$ represent the edges of G. Precisely, each $(u, v) \in E$ defines a unit vector $|u, c\rangle$ for $\mathcal{H}_w$, analogously to how each vertex defines an entry in $\pi(t)$. In this case, $|\Psi(t)\rangle$ is called the state vector of the quantum walk and is computed as

$$|\Psi(t)\rangle = \sum_{v \in V, c \in C_v} \psi(v, c, t) \, |v, c\rangle \, , \tag{2}$$

which gives a superposition of the edges of E. The evolution of the quantum walk is performed by two unitary operators $S(t)$ and $W(t)$ as

$$|\Psi(t)\rangle = S(t)W(t) \, |\Psi(t)\rangle \, , \tag{3}$$

where $S(t)$ and $C(t)$ are respectively named the shift and coin operator. Intuitively, at every instant t, a quantum walk assigns a complex number $\psi(v, c, t)$ to each edge of G, which encodes the probability that the walker is found at that edge as $\rho(v, c, t) = |\psi(v, c, t)|^2$. The coin operator combines these complex numbers among the edges that are incident to the same vertex, while the shift operator moves these quantities to neighbors of a vertex. The probability that the walker is in v at time t is $\upsilon(v, t) = \sum_c \rho(v, c, t)$.

The complete description of quantum and random walks, as well as the definition of Dirac's notation are presented in detail in Chapter 2 of the thesis [Andrade 2020].

3. Matching quantum walks with time-dependent random walks

In order to show that a random walk can be statistically equivalent to a quantum walk, it is necessary to define a time-dependent stochastic matrix $P(t)$ that satisfies the equation

$$\upsilon(t+1) = P(t)\upsilon(t), \tag{4}$$

where the vector $\upsilon(t)$ represents the vertex probability distribution of the quantum walk as defined in Section 2. Note that this theoretical framework is sufficient for establishing the equivalence, since Equation 4 is identical to Equation 1 which describes the evolution of a random walk. The following theorem establishes how $P(t)$ in Equation 4 can be constructed. The proof and details can be found in Chapter 3 of the thesis [Andrade 2020].

Theorem 1. *For any time instant t, the evolution of the vertex probability of a quantum walk performed by the action of the unitary operator SW is local and equivalent to the Markovian matrix $P(t)$ where*

$$p_{vu}(t) = \begin{cases} \frac{\rho(v,c,t+1)}{\upsilon(u,t)}, & \text{if } \upsilon(u,t) > 0 \text{ and } (u,v) \in E \\ \frac{1}{d(u)}, & \text{if } \upsilon(u,t) = 0 \text{ and } (u,v) \in E \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

such that $\pi(t+1) = P(t)\pi(t)$, where $c = \sigma(u,v)$.

Essentially, Theorem 1 determines the evolution of quantum walk vertex probability for a generic time instant. It leverages the fact that both quantum and random walks are Markovian, so that the system at instant $t+1$ is completely described by the system at instant t. Precisely, the construction given in Theorem 1 is possible because the quantum walk wavefunction incident to v in instant $t+1$ is completely determined by the wavefunction incident neighbors of v at time t. This local evolution of the wavefunction is compatible with the evolution of the probability distribution of a random walk, as discussed in Section 2.

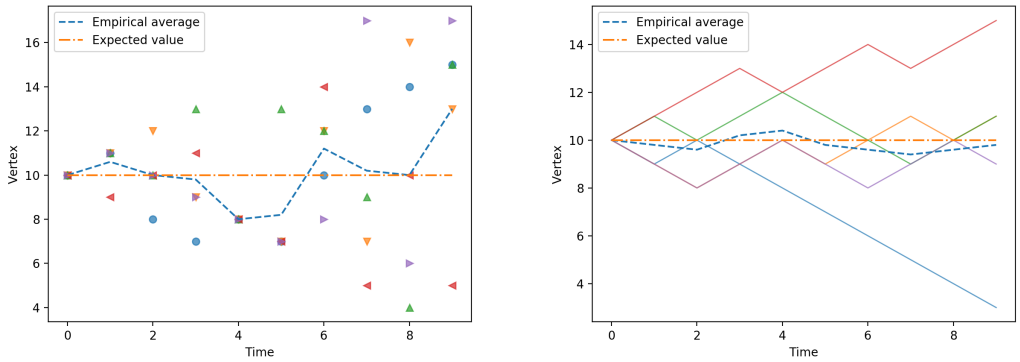
Theorem 1 can be extended to the case of multiple quantum walkers by considering a graph that encodes their joint movement. A node in this graph is a tuple that represents the current position of each of the K walkers, such that $P(t)$ is a $|V|^K$-by-$|V|^K$ stochastic matrix. The possible interactions between the walkers are captured by the edges of this graph, and thus their joint dynamics respect the local evolution of probabilities. The theorem for the multiple walker case, together with its proof and discussion is found in Chapter 3 of the thesis [Andrade 2020].

Note that the exponential growth of $P(t)$ with the number of walkers indicates that multiple interacting quantum walkers cannot be efficiently described by random walks, in contrast with the single walker case. This result is expected due to the hardness of simulating physical quantum systems with multiple particles, which is one of the main motivations for building quantum computers.

3.1. Quantum walk trajectories

The simulation of quantum and random walks is fundamentally different: quantum walks are simulated by a measurement at an specific time instant, such that samples for sequential time instants do not necessarily yield a path in the graph. On the other hand, random walks are usually simulated by generating sample paths, which can be done very efficiently. These differences are described in more detail in Chapter 2 of the thesis [Andrade 2020].

In spite of these differences, a direct consequence of Theorem 1 is a method to simulate a random walk that has the exact same vertex distribution of a corresponding quantum walk. The simulation of the random walk generates a path in the graph, that captures the following property of the quantum system: when the number of independent paths sampled tends to infinity, the marginal distribution of vertices in the path for time instant t converges to the vertex distribution of the quantum walk for t. This path sample is called a *quantum walk trajectory* since it encodes properties of the quantum walk. Note



(a) Independent measurements. **(b) Quantum walk trajectories**

Figure 1. Comparison between independent and random walk sampling of a Hadamard walk on a cycle with 20 vertices for 10 time steps with initial condition $|\Psi(0)\rangle = \frac{1}{\sqrt{2}}(|10,0\rangle + i\,|10,1\rangle)$.

that quantum walk trajectories can be sampled efficiently with the corresponding random walk. More details are provided in Chapter 4 of the thesis.

The comparison between the traditional quantum walk simulation and the quantum walk trajectories method is depicted in Figure 1, where a Hadamard quantum walk on a 20-vertex cycle is simulated for 10 consecutive time steps. In Figure 1(a), points with the same marker style and color represent a sequence of samples (measurements). When consecutive samples of the same style and color differ from more than one unit in vertex value (y-axis), the vertices are not neighbors of each other. Note that consecutive samples of the same sequence are not necessarily neighbors in the left figure, while every sequence in the right figure correspond to a path of the graph.

4. Matching random walks with quantum walks in unitary evolution

Can a quantum walk match the dynamics of a given random walk on a finite graph? Note that Theorem 1 shows how a random walk can imitate the dynamics of a quantum walk. What about the opposite? If the quantum walk is measured at every time step, then the answer is trivial because the quantum walk collapses to a random walk. Thus, the question is more interesting under the assumption that the quantum system will be measured only at the desired time instant.

Indeed, this can be accomplished by representing the probability vector of the random walk in the Hilbert space of a quantum walk, such that $\upsilon(v,t) = \pi_v(t)$, and by describing shift and coin operators that evolve the quantum walker system following the evolution determined by the stochastic matrix $P(t)$ of the random walk. The following theorem provides a procedure showing that this construction is possible for any random walk on a finite graph. More details and the proof are shown in Chapter 5 of the thesis [Andrade 2020].

Theorem 2. *Let $P(t)$ be a stochastic matrix that defines the evolution of a random walk on a graph G, such that, for all t, $\pi(t+1) = P(t)\pi(t)$. For every instant t, the quantum*

walk with state

$$|\Psi(t)\rangle = \sum_{v\in V, c\in C_v} e^{i\theta(u,\sigma^{-1}(u,v),t-1)}\sqrt{p_{vu}(t-1)}\sqrt{\pi_u(t-1)}\,|v,c\rangle\,, \tag{6}$$

fixed shift operator $S(t) = S_{RW}$ and coin operator $W(t)$ constructed through the Grand-Schmidt procedure , evolves according to

$$|\Psi(t+1)\rangle = S_{RW}W(t)\,|\Psi(t)\rangle\,, \tag{7}$$

such that $\upsilon(u,t) = \pi_u(t)$ and $\upsilon(u,t+1) = \pi_u(t+1)$ for all $u \in V$.

Note that the quantum walk described in Theorem 2 is not measured during its evolution over time. Nonetheless, once measured at time t, the quantum walk will have the same vertex distribution as the corresponding random walk at t. Since Theorem 2 assumes an arbitrary random walk, it can be applied to time homogeneous random walks which exhibit convergence of their probability distribution over time. This result is an important contribution to the literature because it shows that the lack of convergence in the probability distribution of quantum walks demonstrated in the early days was due to the time homogeneity assumption [Aharonov et al. 2001]. Indeed, time dependent quantum walks can be constructed as to have a converging vertex probability distribution, as implied by Theorem 2.

References

Aharonov, D., Ambainis, A., Kempe, J., and Vazirani, U. (2001). Quantum walks on graphs. In *ACM STOC*, pages 50–59.

Aharonov, Y., Davidovich, L., and Zagury, N. (1993). Quantum random walks. *Phys. Rev. A*, 48(2):1687.

Andrade, M. G. (2020). Characterizing the Inherent Relationship Between Unitary Quantum Walks and Non-Homogeneous Random Walks on Finite Graphs. Master's thesis, Federal University of Rio de Janeiro. Available at `https://www.cos.ufrj.br/index.php/pt-BR/publicacoes-pesquisa/details/15/2953`.

Andrade, M. G., Marquezino, F. L., and Figueiredo, D. R. (2020). On the equivalence between quantum and random walks on finite graphs. *Quantum Inf. Process.*, 19(11):1–20.

Andrade, M. G., Marquezino, F. L., and Figueiredo, D. R. (2021). Quantum walks can unitarily match random walks on finite graphs. arXiv pre-print 2103.06463.

Childs, A. M. (2009). Universal computation by quantum walk. *Phys. Rev. Lett.*, 102(18):180501.

Lubasch, M., Joo, J., Moinier, P., Kiffner, M., and Jaksch, D. (2020). Variational quantum algorithms for nonlinear problems. *Phys. Rev. A*, 101:010301.

Montero, M. (2017). Quantum and random walks as universal generators of probability distributions. *Phys. Rev. A*, 95(6):062326.

Portugal, R. (2013). *Quantum walks and search algorithms*. Springer.

Shor, P. W. (1994). Algorithms for quantum computation: discrete logarithms and factoring. In *IEEE FOCS*, pages 124–134.