Quantum Walks with Entangled Coins

S. E. Venegas-Andraca[1], J. L. Ball[1], K. Burnett[1], and S. Bose[2]

[1]University of Oxford, UK, [2] University College London, UK

Introduction

Classical random walks are a fundamental tool in Computer Science due to their use in the development of stochastic algorithms [1]. A notable example is that of the best algorithm known so far for the solution of 3-Satisfiability problem, a fundamental problem in Computer Science. This algorithm is based on random walks techniques [2]. The development of Quantum Computation and Quantum Information has revealed that the exploitation of inherently quantum mechanical systems for computational purposes leads to significant advantages over purely classical systems. In recent years interest in the field of quantum walks, quantum mechanical generalisations of classical random walks, has grown hugely due to the importance of classical random walks in computer science.

In this poster, we present a mathematical formalism for the description of unrestricted quantum walks with entangled coins and one walker. The numerical behaviour of such walks is examined when using a Bell state as the initial coin state, one coin operators, one shift operator, and one walker. We compare and contrast the performance of these quantum walks with that of a classical random walk consisting of one walker and two maximally correlated coins. This work is based on [3].

Classical random walks

For an unrestricted classical random walk starting at position $z_0 = 0$, the probability of finding the walker at position k after n steps, when with probability p the walker takes a step to the right and with probability $q = 1 - p$ takes a step to the left (i.e. tossing the coin with probability p of obtaining outcome T and probability q of obtaining outcome H), is given by

$$P_{ok}^{(n)} = \binom{n}{\frac{1}{2}(k+n)} p^{\frac{1}{2}(k+n)} q^{\frac{1}{2}(n-k)} \tag{1}$$

for $\frac{1}{2}(k+n) \in \{0, 1, \ldots, n\}$ and 0 otherwise.

Tossing a pair of coins produces two discrete random variables C_1 and C_2, and the correlation ρ between these two random variables is given by $\rho(C_1, C_2) = \frac{\text{Cov}(C_1,C_2)}{\sqrt{\text{Var}(C_1)\text{Var}(C_2)}}$ where Cov(X,Y) and Var(X) are the covariance and the variance of the corresponding random variables, and ρ is bounded by $-1 \leq \rho \leq 1$. $\rho(C_1, C_2) = 0$ means that random variables C_1 and C_2 are totally uncorrelated, whereas $\rho(C_1, C_2) = 1$ means that random variables C_1 and C_2 are maximally correlated.

Now consider a classical random walk that has a maximally correlated pair of coins, i.e. $\rho(C_1, C_2) = 1$. Also suppose that the first coin C_1 is unbiased. Then the only two outcomes allowed for this coin pair are $O_1 = (H_1, H_2)$ or $O_2 = (T_1, T_2)$. If O_1 allows the walker to move one step to the left and O_2 allows the walker to move one step to the right, it is then clear that using such a coin pair in a classical random walk would produce a probability distribution equal to that of Eq. (1), with $p = \frac{1}{2}$. Thus the use of maximally correlated unbiased coins in classical random walks is not different with respect to a classical random walk with a single unbiased coin, as the probability distributions from both kinds of classical random walks are exactly the same.

Discrete Quantum Walks on an Infinite Line

Walker and Coin: The walker is a quantum system living in a Hilbert space of infinite but countable dimension $\mathcal{H}_p$. It is customary to use vectors from the computational basis of $\mathcal{H}_p$ as "position sites" for the walker. So, we denote the walker as $|\text{position}\rangle \in \mathcal{H}_p$ and affirm that the computational basis states $|i\rangle_p$ that span $\mathcal{H}_p$, as well as any superposition of the form $\sum_i \alpha_i |i\rangle_p$ subject to $\sum_i |\alpha_i|^2 = 1$, are valid states for $|\text{position}\rangle$. The walker is usually initialized at the 'origin', i.e. $|\text{position}\rangle_{\text{initial}} = |0\rangle_p$.

The coin is a quantum system living in a 2-dimensional Hilbert space $\mathcal{H}_c$. The coin may take the canonical basis states $|0\rangle$ and $|1\rangle$ as well as any superposition of these basis states. Thus $|\text{coin}\rangle \in \mathcal{H}_c$ and a general state of the coin may be written as $|\text{coin}\rangle = a|0\rangle_c + b|1\rangle_c$, where $|a|^2 + |b|^2 = 1$.

The total state of the discrete quantum walk resides in $\mathcal{H}_t = \mathcal{H}_p \otimes \mathcal{H}_c$. Only product states of $\mathcal{H}_t$ have been used as initial states, that is, $|\psi\rangle_{\text{initial}} = |\text{position}\rangle_{\text{initial}} \otimes |\text{coin}\rangle_{\text{initial}}$.

Evolution Operators: The evolution of a discrete quantum walk is divided into two parts that closely resemble the behaviour of a classical random walk. In the classical case, we first toss a coin and then, depending on the coin outcome, the walker moves one step either to the right or to the left. In the quantum case, the equivalent of the previous process is to apply an evolution operator to the coin state followed by a conditional shift operator to the total system.

The purpose of the coin operator is to render the coin state in a superposition, and the randomness is introduced by performing a measurement on the system after both evolution operators have been applied to the total quantum system several times. Among coin operators, customarily denoted by $\hat{C}$, the Hadamard operator has been extensively used:

$$\hat{H} = \frac{1}{\sqrt{2}}(|0\rangle_{cc}\langle 0| + |0\rangle_{cc}\langle 1| + |1\rangle_{cc}\langle 0| - |1\rangle_{cc}\langle 1|) \tag{2}$$

For the conditional shift operator use is made of a unitary operator that makes the walker go one step forward if the accompanying coin state is one of the two basis states (e.g. $|0\rangle$), or one step backwards if the accompanying coin state is the other basis state ($|1\rangle$). A suitable conditional shift operator is

$$\hat{S} = |0\rangle_{cc}\langle 0| \otimes \sum_i |i+1\rangle_{pp}\langle i| + |1\rangle_{cc}\langle 1| \otimes \sum_i |i-1\rangle_{pp}\langle i|. \tag{3}$$

Consequently, the operator on the total Hilbert space is $\hat{U} = \hat{S}.(\hat{C} \otimes \mathbb{1}_p)$ and a succint mathematical representation of a quantum walk after n steps is $|\psi\rangle = (\hat{U})^n |\psi\rangle_{\text{initial}}$, where $|\psi\rangle_{\text{initial}} = |\text{position}\rangle_{\text{initial}} \otimes |\text{coin}\rangle_{\text{initial}}$. An example of a discrete quantum walk on an infinite line with evolution operators from Eqs.(2,3) and total initial $|\psi\rangle_{\text{initial}} = |0\rangle_{\text{coin}} \otimes |0\rangle_{\text{walker}}$ is given in Fig.(1).

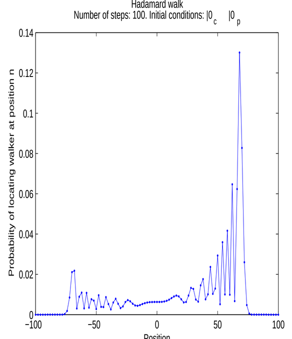

Fig. 1 Discrete quantum walk with evolution operators from Eqs.(2,3) and total initial $|\psi\rangle_{\text{initial}} = |0\rangle_{\text{coin}} \otimes |0\rangle_{\text{walker}}$

Mathematical Structure of Quantum Walks on an Infinite Line Using a Maximally Entangled Coin

Walker and Coin: The walker is, as in the unrestricted quantum walk with a single coin, a quantum system $|\text{position}\rangle$ residing in a Hilbert space of infinite but countable dimension $\mathcal{H}_P$. The canonical basis states $|i\rangle_P$ that span $\mathcal{H}_P$, as well as any superposition of the form $\sum_i \alpha_i |i\rangle_P$ subject to $\sum_i |\alpha_i|^2 = 1$, are valid states for the walker. The walker is usually initialized at the 'origin' i.e. $|\text{position}\rangle_0 = |0\rangle_P$.

The coin is now an entangled system of two qubits i.e. a quantum system living in a 4-dimensional Hilbert space $\mathcal{H}_{EC}$. We denote coin initial states as $|\text{coin}\rangle_0$. Also, we shall use the following Bell states as coin initial states $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, $|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$, and $|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ which are maximally entangled pure bipartite states with reduced von Neumann entropy equal to unity. The Bell singlet state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ is not employed as an entangled coin as it is left invariant when the same local unitary operator is applied to both coins.

The total initial state of the quantum walk lives in $\mathcal{H}_T = \mathcal{H}_P \otimes \mathcal{H}_{EC}$: $|\psi\rangle_0 = |\text{position}\rangle_0 \otimes |\text{coin}\rangle_0$

Evolution Operators: The evolution operators used are more complex than those for quantum walks with single coins. As in the single coin case, evolution operators must be unitary.

Let us start by defining evolution operators for an entangled coin. Since the coin is a bipartite system, its evolution operator is defined as the tensor product of two single-qubit coin operators: $\hat{C}_{EC} = \hat{C} \otimes \hat{C}$. For example, we could define the operator $\hat{C}_{EC}^H$ as the tensor product $\hat{H}^{\otimes 2}$:

$$\begin{aligned}\hat{C}_{EC}^H = \frac{1}{2}(&|00\rangle\langle 00| + |01\rangle\langle 00| + |10\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 01| - |01\rangle\langle 01| + |10\rangle\langle 01| - |11\rangle\langle 01| \\ &+ |00\rangle\langle 10| + |01\rangle\langle 10| - |10\rangle\langle 10| - |11\rangle\langle 10| + |00\rangle\langle 11| - |01\rangle\langle 11| - |10\rangle\langle 11| + |11\rangle\langle 11|).\end{aligned} \tag{4}$$

An alternative bipartite coin operator is produced by computing the tensor product $\hat{Y}^{\otimes 2}$ where $\hat{Y} = \frac{1}{\sqrt{2}}(|0\rangle\langle 0| + i|0\rangle\langle 1| + i|1\rangle\langle 0| + |1\rangle\langle 1|)$, namely

$$\begin{aligned}\hat{C}_{EC}^Y = \frac{1}{2}(&|00\rangle\langle 00| + i|01\rangle\langle 00| + i|10\rangle\langle 00| - |11\rangle\langle 00| + i|00\rangle\langle 01| + |01\rangle\langle 01| - |10\rangle\langle 01| + i|11\rangle\langle 01| \\ &+ i|00\rangle\langle 10| - |01\rangle\langle 10| + |10\rangle\langle 10| + i|11\rangle\langle 10| - |00\rangle\langle 11| + i|01\rangle\langle 11| + i|10\rangle\langle 11| + |11\rangle\langle 11|).\end{aligned} \tag{5}$$

The conditional shift operator $\hat{S}_{EC}$ necessarily allows the walker to move either forwards or backwards along the line, depending on the state of the coin. The operator

$$\begin{aligned}\hat{S}_{EC} = &|00\rangle_{cc}\langle 00| \otimes \sum_i |i+1\rangle_{pp}\langle i| + |01\rangle_{cc}\langle 01| \otimes \sum_i |i\rangle_{pp}\langle i| \\ &+ |10\rangle_{cc}\langle 10| \otimes \sum_i |i\rangle_{pp}\langle i| + |11\rangle_{cc}\langle 11| \otimes \sum_i |i-1\rangle_{pp}\langle i|\end{aligned} \tag{6}$$

embodies the stochastic behaviour of a classical random walk with a maximally correlated coin pair. It is only when both coins reside in the $|00\rangle$ or $|11\rangle$ state that the walker moves either forwards or backwards along the line; otherwise the walker does not move.

The total evolution operator has the structure $\hat{U}_T = \hat{S}_{EC}.(\hat{C}_{EC} \otimes \mathbb{1}_p)$ and a succint mathematical representation of a quantum walk after N steps is $|\psi\rangle = (\hat{U}_T)^N |\psi\rangle_0$, where $|\psi\rangle_0$ denotes the initial state of the walker and the coin.

In order to investigate the properties of unrestricted quantum walks with entangled coins, we have computed simulations using bipartite maximally entangled coin states described by the Bell states aforementioned, and coin evolution operators described by Eq.(4,5). Initial position state of the walker is $|\text{position}\rangle_0 = |0\rangle$, and the shift operator employed is that of Eq.(6).

We discuss the quantum walks whose graphs are shown in Fig.(2). The initial entangled coin state is given by Bell state $|\Phi^+\rangle$ and the number of steps is 100. For the red plot in Fig.(2) the coin operator is given by Eq. (4), while for the dotted blue plot in the same Fig. (2) the coin operator is that of Eq. (5).

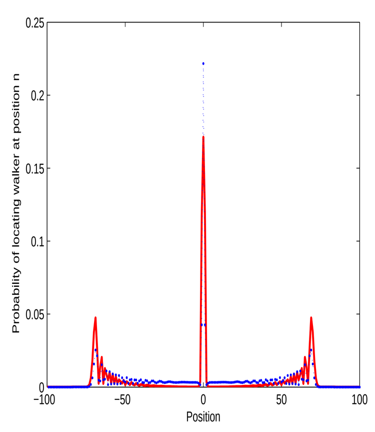

Fig. 2. For both plots, coin initial state is $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ and the number of steps is 100. Coin operators for red and dotted blue plots are given by Eq. (4) and Eq. (5) respectively.

The first notable property of these quantum walks is that, unlike the classical case in which the most probable location of the walker is at the origin and the probability distribution has a single peak, in the quantum case a certain range of very likely positions about the position $|0\rangle$ is evident but in addition there are a further two regions at the extreme zones of the walk in which it is likely to find the particle. This is the 'three peak zones' property of the shift operator defined in this way. The 'three peak zones' property could mean an additional computational advantage of quantum walks over classical random walks (for example, let us suppose we want to design algorithms whose purpose is to find the wrong values in a proposed solution of a problem. If the number of wrong values is in the range 40 - 70, the probability of finding the quantum walker of Fig. (2) is much higher than finding the classical walker of Eq.(1).)

We also note that the probability of finding the walker in the most likely position, $|0\rangle$, is much higher in the quantum case (~ 0.171242 in red plot of Fig. (2) and ~ 0.221622 in dotted blue plot of Fig. (2) than in the classical case (~ 0.0795). Incidentally, we find that the use of different coin initial states maintains the basic structure of the probability distribution, unlike the quantum walk with a single coin in which the use of different coin initial states can lead to different probability distributions.

References

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