Quantum interchange walk as a unifying approach

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Abstract. We construct a quantum interchange walk, related to classical walks with memory. This gives us a coinless discrete walk, while the origin in classical walks with memory offers the promise of use of existing tools from classical memoried walks. This approach readily reproduces all standard approaches. We briefly discuss its generality and advantages.

1 Introduction

Quantum walks have been introduced into study of quantum computation with the hope of benefits similar to those of classical randomized algorithms. Other than speed, quantum walks may offer different approaches, and are one of the rare alternatives to approaches based on Grover's search and Shor's factoring. Since this research direction was established [1, 2] the field of quantum walks has grown considerably, with development of algorithms [4] and implementation designs [5]. For an excellent early survey see [3].

Standard approaches to quantum walks still follow the ideas of memoryless classical walks. While we are still in the early stages in this field, and there is much to be understood and developed from the basic ideas, it is not too early to approach quantum walks from the point of classical walks with memory: quantum evolution is unitary and reversible, and this is only natural. Also, in computer science memoried and biased approaches are common and beneficial algorithmically.

We propose construction of quantum walks related to their most natural classical counterparts, which are random walks with memory. In Section 3, we start with the observation that the standard Hadamard walk is an analog of a persistent walk. Then in Section 4 we build a quantum walk based on a particular representation of a Markov process with memory. Our approach yields a coinless discrete quantum walk. We discuss its advantages, and show that it contains all other standard approaches.

2 A representation of classical walks with memory

We introduce a specific representation of a classical walk with memory, which we are not aware of in the literature. For concreteness, we construct a persistent walk. As it will be seen, this method can be used equally well to construct other walks with memory.

When considering Markov chains with memory $k > 1$, there are multiple possible approaches. Here we use the Markov tensor of dimension $k+1$, and the probability distribution is of dimension k. Since we look at a persistent walk (memory $k = 2$), our state is a matrix, and is evolved by the 3rd rank Markov tensor. In examples we mostly have in mind a walk over the state space $\{0, 1, \ldots, n-1\}$, often with identified ends. Note that, in this section only, we use the fairly standard probabilistic notation, of operators acting on left.

2.1 Description of the state of the walk

A *persistent walk* is a one-dimensional process where the probability for the next step depends on the direction of the previous one. If the walk has come to the site i from the site $i-1$ (having moved to the right), it has the probability p to continue moving to the right, to the site $i+1$; and the probability $1-p$ to reverse direction, and move back to the site $i-1$. This is a particular case of a classical walk with memory 2.

For a memory 2 classical walk, one way to describe the state is by a pair of indices (i, j), with i being the site the walk came from, and j being the site the walk is on. The Markov operator acts on this state, performing the walk. The probability distribution, after t evolutions, can be represented as a matrix with (i, j) entries, or a matrix of row, or column, vectors

$$\mu(t) = \begin{bmatrix} \mu_{0,0}(t) & \cdots & \mu_{0,n-1}(t) \\ \vdots & & \\ \mu_{n-1,0}(t) & \cdots & \mu_{n-1,n-1}(t) \end{bmatrix} = \begin{bmatrix} r_0 \\ \vdots \\ r_{n-1} \end{bmatrix} = \begin{bmatrix} c_0 & \cdots & c_{n-1} \end{bmatrix} \tag{1}$$

where r_j and c_j are respectively row and column vectors of μ (their explicit time dependence has been omitted only for brevity of notation). Each row vector r_j contains probability distribution for a step *from* site j to any other; while each column c_j carries the distribution for steps having come *to* site j, from all other sites. This will be important for our construction.

Note that all transitions are of the form $(i, j) \to (j, k)$, and that, for the nearest-neighbor walks which we consider, the state can only be one of the $(j \pm 1, j)$, and the transition can only be made to a $(j, j \pm 1)$ state.

2.2 A representation of the Markov tensor

The evolution operator can be represented as n layers of $n \times n$ transition matrices P_j, each associated with one state. Let $p_{ij|k}$ be the conditional probability for the transition $j \to k$, given that the walk came to j from i. All such transition probabilities $\{p_{ij|k}\}$ define the evolution operator, $\mathcal{M} = [P_0 P_1 \dots P_{n-1}]$, where for each j we have

$$P_j = \begin{bmatrix} p_{0,j|0} & p_{0,j|1} & \cdots & p_{0,j|n-1} \\ \vdots & & & \vdots \\ p_{n-1,j|0} & p_{n-1,j|1} & \cdots & p_{n-1,j|n-1} \end{bmatrix}, \quad j = 0, 1, \dots, n-1 \qquad (2)$$

Each P_j is by construction indeed a transition probability matrix. Such a P_j transition matrix acts on the (transposed) j-th column of the distribution matrix $\mu(t)$, resulting in the j-th row of $\mu(t+1)$. The evolution of the state, $\mu(t+1) = \mu(t) \cdot \mathcal{M}$, is then defined as

$$\mu(t) \mapsto \mu(t+1) \; : \; r_j(t+1) = c_j^\top(t) P_j, \text{ for each } j = 0, 1, \dots, n-1 \qquad (3)$$

where r_j and c_j are j-th row and column respectively, of the matrix μ. Thus P_j act on transposed columns of $\mu(t)$, giving rows for $\mu(t+1)$.

Note the meaning of this construction: the P_j matrices carry probabilities to move from j to any other site, while the j-th column of μ has the probabilities to have come to j from any site. Then the action of P_j on the j-th column (transposed) yields distribution of probabilities to have come to the j-th site from all possible sites, and to have moved on to all possible sites, ie. the j-th row of the evolved state. Thus action of all transition matrices on all columns evolves the probability distribution over all paths.

For example, consider a persistent walk on the cycle of n sites, with identified ends. Then the P_j matrices have the following block centered at $(j,j) \pmod{n}$:

$$\begin{array}{c|c} & \begin{array}{ccccc} & {\scriptstyle (j-1)} & {\scriptstyle (j)} & {\scriptstyle (j+1)} & \end{array} \\ \begin{array}{c} \\ {\scriptstyle (j-1)} \\ {\scriptstyle (j)} \\ {\scriptstyle (j+1)} \\ \\ \end{array} & \begin{bmatrix} \ddots & & & & \\ & 1-p & 0 & p & \\ & 0 & 1 & 0 & \\ & p & 0 & 1-p & \\ & & & & \ddots \end{bmatrix} \end{array} \qquad \text{indices are mod}(n) \qquad (4)$$

They also have 1 on the diagonal, with other elements 0, except for the ones dealing with the boundary conditions. For example, take identified ends, and consider the above block for $P_{j=0}$. The entry at $(j-1, j-1)$ (which is $1-p$), is at $(-1,-1)$, and this is $(n-1, n-1)$, since $n \leftrightarrow 0$. The $(j+1, j-1)$ entry $(=p)$ is at $(1, n-1)$, etc.

This representation of the Markov evolution offers very interesting uses in studies of classical stochastic processes. It also lends itself to an approach in construction of quantum walks.

3 Quantum walks are memoried

One of the deepest requirements of quantum mechanics is unitarity; quantum evolution has memory. Still, quantum walks have mostly been built following an analogy with classical memoryless walks. Here we establish that, instead, a classical walk with memory is a natural classical analog of a quantum walk. We build a walk using a generalized Hadamard gate, as an analog of a persistent classical walk; and a more general walk using the interchange circuit, corresponding to classical walks with memory.

In this Section we address 'coined' quantum walks, and show that they are a natural analog of persistent walks. We review the construction from [2], and then, using different probabilities to take steps in different directions, show that the standard coin–walks have a natural correspondence with classical persistent walks. In the next Section we introduce a more general mechanism for building a quantum walk, that directly relates to a classical walk with memory 2, and contains the coined walks. We will see that Grover and Szegedy walks are also analogs of memory 2 walks.

3.1 Quantum walk from a memoryless classical walk

For further reference and comparison, here we briefly summarize the construction of a walk on a d-regular graph with n vertices, from [2]. The state is in the following direct product of two spaces. The first subspace, $\mathcal{H}_A$, is the 'coin space,' an auxiliary Hilbert space spanned by d states $|a\rangle$; a unitary operator C acting in this space represents a 'coin toss.' The second is the space of vertices, $\mathcal{H}_V$, spanned by n states $|v\rangle$. The evolution operator acts in the space $\mathcal{H}_A \otimes \mathcal{H}_V$ as: $U(|a\rangle \otimes |v\rangle) = S \cdot (C \otimes I)(|a\rangle \otimes |v\rangle)$. In the case of a cycle with n nodes, for the coin toss one can use the Hadamard transform

$$C \;=\; \mathbf{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{5}$$

and after its action the graph (circle) is then shifted by the operator S. Then the walk is a repeated application of the operator $U = S \cdot (C \otimes I)$.

An implementation for S on a cycle, following up on the action of C, is: $S = |\uparrow\rangle\langle\uparrow| \otimes \sum_j |j+1\rangle\langle j| + |\downarrow\rangle\langle\downarrow| \otimes \sum_j |j-1\rangle\langle j|$. The first factor in each term selects the part of the state that is either in the 'up' or 'down' direction of the coin (arbitrarily taken to mean right of left), the second projector shifts that state accordingly.

In order to see how the eigenproblem is approached, and for future reference, let us write out the evolution step. Apply U to the state of the coin $|c\rangle = \sum_1^d c_a|a\rangle$, with $|a\rangle$ being the coordinate vectors in the coin space $\mathcal{H}_A$; the state vector in the space of vertices is labeled $|v\rangle$. Then $U|c,v\rangle = S\cdot(C|c\rangle \otimes |v\rangle) = S \cdot \sum_1^d c_a|a\rangle \otimes |v\rangle$. The matrix S can in general be constructed as $S = \sum_1^d |a\rangle\langle a| \otimes S_a$, where S_a is the shift along a. Then, given that the operators above act in the product spaces only

$$U|c,v\rangle = \sum_{a=1}^{d} |a\rangle\langle a| \otimes S_a \cdot \left(\sum_{a=1}^{d} c_a|a\rangle \otimes |v\rangle \right) = \sum_{a=1}^{d} c_a|a\rangle \otimes S_a|v\rangle \tag{6}$$

The shift performed by S_a is the group action, $S_a|v\rangle = \chi(g_a^{-1})|v\rangle$, where $\chi(g_a^{-1})$ is the character of the group element g_a, and its inverse is used since the graph is shifted, [2]. Then $U|c,v\rangle = (\sum_1^d \chi(g_a^{-1})\, c_a|a\rangle) \otimes |v\rangle$. This means that we need eigenvectors for the operator $\mathbf{H}_k = \Lambda_k \cdot C$, where $\Lambda_k(a,a) = \mathrm{diag}\{\chi(g_a^{-1})\}$ and k labels the representation. For the cycle, with $w^k = e^{\frac{2\pi i}{n}k}$, this is

$$\mathbf{H}_k = \Lambda_k \cdot C = \begin{bmatrix} w^k & 0 \\ 0 & w^{-k} \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{w^k}{\sqrt{2}} & \frac{w^k}{\sqrt{2}} \\ \frac{w^{-k}}{\sqrt{2}} & -\frac{w^{-k}}{\sqrt{2}} \end{bmatrix} \tag{7}$$

As the construction of $\mathbf{H}_k$ includes the action of S, this matrix is a representation of the whole operator U, in the coordinate basis $\{|a_i\rangle, |v_i\rangle\}$. The choice of fixed and equal factors in $\mathbf{H}$ yields an unbiased walk. We will see below that this is a special case of a quantum interchange walk.

3.2 Quantum Hadamard walk and persistent classical walk

Now we discuss a straightforward generalization of the unbiased quantum walk. With the exact construction of the previous example, using unequal probabilities for different directions of the walk (of p and $1-p$), we get a quantum walk that is persistent in nature, and in its pure states represents a quantum analog of a persistent classical walk.

To see this, look at a step with the general Hadamard coin operator

$$C = \begin{bmatrix} \sqrt{p} & \sqrt{1-p} \\ \sqrt{1-p} & -\sqrt{p} \end{bmatrix} \tag{8}$$

starting from the initial pure state. First we look at the state with the coin 'up,' for the walk moving to the right. With an appropriate shift following the action of C above, for the initial state $|\uparrow\rangle \otimes |i\rangle$, the evolution step is

$$|\uparrow\rangle \otimes |i\rangle \xrightarrow{S\cdot(C\otimes I)} \begin{cases} (\sqrt{p})\ |\uparrow\rangle \otimes |i+1\rangle & \text{(continues moving right)} \\ (\sqrt{1-p})\ |\downarrow\rangle \otimes |i-1\rangle & \text{(changes direction to left)} \end{cases}$$

for the previous step taken to the right. Thus the evolution operator $S \cdot (C \otimes I) = (\sum_{a=1}^{d} |a\rangle\langle a|S_a) \cdot (C \otimes I)$ acts as

$$\begin{aligned} S \cdot (C \otimes I)\,|\downarrow\rangle \otimes |i\rangle &= S \cdot \left(\sqrt{p}\ |\uparrow\rangle \otimes |i\rangle + \sqrt{1-p}\ |\downarrow\rangle \otimes |i\rangle\right) \\ &= \sqrt{p}\ |\uparrow\rangle \otimes |i+1\rangle + \sqrt{1-p}\ |\downarrow\rangle \otimes |i-1\rangle \end{aligned} \tag{9}$$

Similarly, take a step from a pure initial state with the coin down, $|c\rangle_d = [\,0,\ 1\,]^{\mathsf{T}}$, representing the walker moving to the left, $i \to i-1$. The action of the coin operator gives $C\,|c\rangle_d = \left[\sqrt{1-p},\ -\sqrt{p}\right]^{\mathsf{T}}$ and then the shift operator completes the transition to the new state

$$\begin{aligned} S \cdot (C \otimes I)\,|\downarrow\rangle \otimes |i\rangle &= S \cdot \left(\sqrt{1-p}\ |\uparrow\rangle \otimes |i\rangle - \sqrt{p}\ |\downarrow\rangle \otimes |i\rangle\right) \\ &= \sqrt{1-p}\ |\uparrow\rangle \otimes |i+1\rangle - \sqrt{p}\ |\downarrow\rangle \otimes |i-1\rangle \end{aligned} \tag{10}$$

We see a walk mimicking a classical persistent walk, when starting from pure states: it continues moving in the same direction with the probability p (obtained by squaring the amplitude), while it changes the direction with the probability $1-p$. In mixed states, the action is the same on each component.

Using the periodicity of the cycle, and the identification of n sites on the circle by the roots of unity $w^k = e^{\frac{2\pi i}{n}k}$, we have $|i+1\rangle = w^{-k}|i\rangle$. The evolution $U|c, v\rangle$ of Eq.s (9) and (10) can then be represented as

$$S \cdot (C \otimes I)\,|c\rangle \otimes |v\rangle = \frac{1}{\sqrt{N}} \begin{bmatrix} w^k\sqrt{p} & w^k\sqrt{1-p} \\ w^{-k}\sqrt{1-p} & -w^{-k}\sqrt{p} \end{bmatrix} |c\rangle \otimes |v\rangle \tag{11}$$

We have the same eigenvalue problem as in the reviewed unbiased example of [2], but yielding a clear interpretation of a persistent walk. Our eigenvalues are of course different, offering some interesting analysis, but the main theorems of [2] hold for this walk.

Note that the directionality of the walk is naturally present: it came at no cost as soon as the coin transformation is allowed to have probabilities other than $p = 0.5$. In other words, the standard Hadamard transform, Eq. (5), does not implement a memoryless walk, but is rather a persistent walk (only with equal probabilities). This is unsurprising for a quantum system, with its unitary evolution.

After this straightforward discussion of coined walks, we look at a more general construction of a quantum walk with memory, using our method from Section 2.

4 Quantum interchange walk

We construct a quantum walk of memory 2, using a more general approach, presented in Section 2 for a classical Markov evolution. The probability distribution is in the product of spaces, of sites and internal states:

$$|\xi(t)\rangle = \xi_{ij}(t)\,|i\rangle \otimes |j\rangle, \quad \text{over } \mathbb{C}^N \times \mathbb{C}^N \tag{12}$$

We use the interchange circuit, $\hat{X}\colon\ |i\rangle \otimes |j\rangle \mapsto |j\rangle \otimes |i\rangle$. This transformation can be implemented with CNOT gates, when applied successively to qubits. Then, with U being unitary transformations in $\mathbb{C}^N$,

$$|\xi(t+1)\rangle = (UX)|\xi(t)\rangle, \quad \text{and} \quad |\xi(t)\rangle = (UX)^t\,|\xi(0)\rangle \tag{13}$$

Here the evolution transformation (algorithm) U acts in $\mathbb{C}^N$ as:

$$U = \sum_{j=1}^{N} \mathit{\Pi}_j \otimes U_j, \quad \text{where} \quad \mathit{\Pi}_j = |j\rangle\langle j| \tag{14}$$

where the $\mathit{\Pi}_j$ selects the first qubit, and U_j acts on the second.

One of the crucial points in this construction is that there is no coin. The dynamics of the evolution is based on the interplay of the interchange transformation and U_j matrices. The interchange forces the walk forward, 'reversing the arrow,' without deciding where the walk steps; then, the stochastic nature of the walk is carried out by the U_j transformation matrices, which 'rotate the arrow' toward the site for the next step. This eliminates the need for a coin altogether. A visual representation of a step can be

$$\underset{i}{\bullet} \rightarrow \underset{j}{\bullet} \quad \overset{\hat{X}}{\longmapsto} \quad \underset{i}{\bullet} \leftarrow \underset{j}{\bullet}, \qquad \text{and } U_j \text{ rotates the tip to } k: \quad j \bullet \nearrow \bullet\, k$$

We emphasize that this allows for different transformations to be assigned for different sites. Also note that probabilities p in $U_j(p)$, in the forthcoming example of Eq. (15), may too be set at every step differently, so that the dynamics can be manipulated step to step, via assignments $U_j(p)$. This offers flexibility in construction of walks using this method.

4.1 Coin walks are a case of quantum interchange walks

Here we show that coined walks are an example of interchange walks. The above general approach of interchange walks can be used to construct persistent walks, thus reproducing coined walks. This will also serve as a specific example of the construction. A representation for U_j follows from the construction for a classical memoried walk from Section 2, Eq. (4)

$$U_j(p) \;=\; \begin{bmatrix} \ddots & & & & \\ & \sqrt{1-p} & 0 & \sqrt{p} & \\ & 0 & 1 & 0 & \\ & -\sqrt{p} & 0 & \sqrt{1-p} & \\ & & & & \ddots \end{bmatrix} \tag{15}$$

The square roots provide for the probability, in quantum systems being the square of the amplitude; the $-\sqrt{p}$ sign is necessary to have U_j unitary. Other entries are much like in the classical case: 1's on the diagonal, zeros almost everywhere else, except for entries necessary to honor boundary conditions.

To look at the walk this generates, act with $\hat{U}\hat{X}$ on a pure state. First, look at the state $|i-1\rangle \otimes |i\rangle$, having in mind a persistent walk: the walk is on the site i, having moved to the right, from the site $i-1$. Using the above construction for U_j matrices

$$\hat{U} \cdot \hat{X}\, |i-1\rangle \otimes |i\rangle \;=\; \sqrt{1-p}\; |i\rangle \otimes |i-1\rangle \;+\; \sqrt{p}\; |i\rangle \otimes |i+1\rangle \tag{16}$$

When acting on the walk directed opposite, in the pure state $|i+1\rangle \otimes |i\rangle$,

$$\hat{U} \cdot \hat{X}\, |i+1\rangle \otimes |i\rangle \;=\; -\sqrt{p}\; |i-1\rangle \otimes |i\rangle \;+\; \sqrt{1-p}\; |i+1\rangle \otimes |i\rangle \tag{17}$$

Such evolution of pure states maintains the interpretation of a persistent walk: with the probability $1-p$ the walker reversed direction, and with the probability p it continued. Since the operators U_j are linear and probability operators, and the walk stays in the subspace of adjacent sites, we can assert that an arbitrary mixed state evolves according to the above analysis, as a directed walk.

Note that this is an isomorphism of the example of the unbiased walk, of Eq.s (9) and (10), via identifications

$$|i-1\rangle \otimes |i\rangle \Leftrightarrow |\uparrow\rangle \otimes |i\rangle \quad \text{and} \quad |i+1\rangle \otimes |i\rangle \Leftrightarrow |\downarrow\rangle \otimes |i\rangle \tag{18}$$

The quantum interchange walk constructed above contains the persistent walk implemented with Hadamard transformation with $p \neq 0.5$. Similarly, any coined walk can be reproduced.

4.2 Grover walk from quantum interchange walk

By a suitable choice of the transformation matrices U_j other standard quantum walks can be obtained. Consider a process on the irregular graph. Let the order of vertex j be d_j, and let its neighboring vertices be $i_1, \ldots, i_{d_j}$. For each vertex, its order d_j and neighbors $\{i_{d_j}\}$ define the transformation matrix U_j

$$U_j \;=\; \begin{array}{c} \\ i_1 \\ \vdots \\ i_{d_j} \\ \\ \end{array} \overset{\displaystyle \begin{array}{ccc} i_1 & \cdots & i_{d_j} \end{array}}{\begin{bmatrix} \ddots & & & & \\ & \frac{2}{d_j}-1 & \frac{2}{d_j} & \frac{2}{d_j} & \\ & \frac{2}{d_j} & \frac{2}{d_j}-1 & \frac{2}{d_j} & \\ & \frac{2}{d_j} & \frac{2}{d_j} & \frac{2}{d_j}-1 & \\ & & & & \ddots \end{bmatrix}} \tag{19}$$

The block above is $d_j \times d_j$. The remaining diagonal elements of the matrix are 1, the rest are 0.

The evolution of the interchange walk, via Eq.s (13) and (14), performed with the above construction of matrices associated with each vertex, is Grover diffusion, introduced in [6]. Similarly, the appropriate choice of U_j matrices nicely reproduces Szegedy walk.

5 Summary and discussion

We have shown that Hadamard, Grover, and other quantum walks are naturally related to memoried walks. For example, the standard Hadamard walk is not really an analog of a memoryless walk, but it is rather a persistent walk, which is apparent as soon as probabilities for steps are relaxed to be $p \neq 0.5$.

We propose approaching quantum walks from memoried classical ones. We present one such construction, following our particular representation of a classical Markov evolution. The walk built this way has no coin: the interchange transformation prepares the walk (by ‘reversing the arrow’), and then the U_j transition matrices decide about and perform the next step (by ‘rotating the arrow’ to the next site), thus carrying the walk’s stochastic character. This brings various advantages.

We have shown how the interchange walk contains other approaches, both coined and Grover–style walks. A much greater variety of processes can be modeled, and walks constructed, by way of assignments of U_j for each site. Take for example $U_j = U_j(p_j)$ in Eq. (15), and vary p_j at every site. Also note that the adjustment of probabilities p_j at various steps (with time), as needed, opens yet other venues. This approach is extremely flexible, and there seem to be nearly no limit to what can be constructed with it.

Since there is no coin, there is not much in the way of relating continuous and discrete walks with this approach, for example by simply slowing down the walk.

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