Reflections in Hilbert Space IV: Quantum walks via Szegedy's scheme

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> You can seek any knowledge on demand. How much more productive would humanity be if we can achieve this? –*Amit Singhal, Googles Search Lead*

In the final lecture, we focus on discrete time quantum walks and their connection to the reflection operations we've been considering so far in the series. Discrete time quantum walks were an outpouring of the study of quantum cellular automata [1, 2] and were first seriously recognized as useful for quantum speedup in the paper by Ambainis [3]. Ref. [3] was the precursor to Szegedy's work [4, 5] that we've been discussing in the previous lectures. There are many different applications of discrete time quantum walks as discussed in reviews [6, 7, 8] and to close the lecture we will discuss a recent paper [9] on simulating Google's PageRank algorithm using discrete time quantum walks.

The lecture begins with discrete quantum walks on a line followed by the generalization to discrete quantum walks on general graphs, and, finally, the quantized Google PageRank algorithm. The aim of the presentation is to impart a broad understanding of discrete quantum walks as the products of reflection operators; just as we've been studying.

Throughout the lecture, the Hilbert space will be partitioned into two spaces, e.g. $\mathcal{H}_A \otimes \mathcal{H}_B$ and the following two notations are used interchangeably for matrix elements (rank one projectors):

$$|a, b\rangle\langle\alpha, \beta| = |a\rangle\langle\alpha| \otimes |b\rangle\langle\beta|$$

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1 Discrete time quantum walks

1.1 Discrete quantum walks on a line

Classically, discrete and continuous time walks treat time differently, but the vertex space, $\mathcal{H}_V$, of both types of walks are the same. Quantum mechanically, this is not the case and the state space of the discrete time quantum walk must be enlarged to support non-trivial unitary dynamics.

Meyer proved [1] that if a rule for discrete time quantum evolution is the same for each site and depends on some local neighborhood of that site then there is no non-trivial unitary matrix. Specifically, if a unitary matrix is banded with a width of r entries and commutes with one-step translation operator in (1) then it is must also be a translation operator to some power times a phase. Thus, the two following operators are special as they are the only unitary operators (up to a phase) on an infinite line satisfying locality and translation invariance.

$$S_+ = \sum_{n=-\infty}^{\infty} |n+1\rangle\langle n| \tag{1}$$

$$S_- = \sum_{n=-\infty}^{\infty} |n-1\rangle\langle n| = (S_+)^\dagger \tag{2}$$

This limitation is circumvented by using an extra degree of freedom frequently called a "coin" when this extension is two-dimensional. As a result, the auxiliary space is denoted $\mathcal{H}_C$.

The unitary evolution on the enlarged space, $\mathcal{H}_V \otimes \mathcal{H}_C$, is done by first, "flipping" the coin then shifting forward or backward based on the state of the coin [1]. Alternatively, we could think of "rotating" the coin. By flipping a 2D coin, we mean that a reflection operation (about some arbitrary) state has been performed, and by rotating a coin, we mean a rotation operation has been performed on the coin. Naturally, we focus on the reflections.

The reflection operator about an arbitrary state, $|f_\pm\rangle = \cos\omega|+\rangle + e^{i\varphi}\sin\omega|-\rangle$, gives

$$2|f_\pm\rangle\langle f_\pm| - \mathbf{1} = 2\begin{bmatrix} \cos^2\omega|-\rangle\langle-| & \frac{1}{2}e^{i\varphi}\sin 2\omega|-\rangle\langle+| \\ \frac{1}{2}e^{-i\varphi}\sin 2\omega|+\rangle\langle-| & \sin^2\omega|+\rangle\langle+| \end{bmatrix} - \mathbf{1} \tag{3}$$

$$= \begin{bmatrix} (2\cos^2\omega - 1)|-\rangle\langle-| & e^{i\varphi}\sin 2\omega|-\rangle\langle+| \\ e^{-i\varphi}\sin 2\omega|+\rangle\langle-| & (2\sin^2\omega - 1)|+\rangle\langle+| \end{bmatrix} \tag{4}$$

$$= \begin{bmatrix} \cos 2\omega|-\rangle\langle-| & e^{i\varphi}\sin 2\omega|-\rangle\langle+| \\ e^{-i\varphi}\sin 2\omega|+\rangle\langle-| & -\cos 2\omega|+\rangle\langle+| \end{bmatrix} \tag{5}$$

[1] This is similar to spin-dependent shifts of neutral atoms (e.g. rubidium or cesium) in optical lattices where the spin of the atom can be rotated using microwaves and then the potential shifts depending on the orientation of the spin. If the spin is in a coherent superposition, then the shift of the atom is also coherently done, see e.g. [10]. This analogy holds for the one dimensional walk but it will not hold in the generalizations considered here.

Using $\varphi = 0$ and $\omega = \theta/2$ in the definition of $|f_\pm\rangle$, [2] we have

$$F^{(n)}(\theta) = 2|f_\pm\rangle\langle f_\pm| - \mathbf{1} = \left[\begin{array}{cc} \cos\theta|-\rangle\langle-| & \sin\theta|-\rangle\langle+| \\ \sin\theta|+\rangle\langle-| & -\cos\theta|+\rangle\langle+| \end{array} \right]. \tag{6}$$

This is our reflection operator at each individual site. The full reflection operator is

$$\begin{aligned} F_C(\theta) &= \sum_n (|n\rangle\langle n| \otimes F^{(n)}(\theta)) && (7) \\ &= 2\sum_n |n, f_\pm\rangle\langle n, f_\pm| - \sum_n |n\rangle\langle n| \otimes \mathbf{1}_\pm && (8) \\ &= 2\sum_n |n, f_\pm\rangle\langle n, f_\pm| - \mathbf{1} \otimes \mathbf{1}_\pm && (9) \end{aligned}$$

Note that $\pi/4$ gives the Hadamard transformation and $\pi/2$ flips the coin from $\pm$ to $\mp$.

A rotation in SU(2) is given by:

$$T(\theta) = \left[\begin{array}{cc} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{array} \right] = \exp[i\theta\sigma^y] \tag{10}$$

The rotation is related to a reflections using the Pauli σ^z matrix as $F^{(n)}(\theta) = \sigma^z T(\theta)$ or through $F^{(n)}(\theta)F^{(n)}(2\theta) = T(\theta)$.

The coin-dependent shift, S, is given by

$$S = \sum_{n=-\infty}^{\infty} |n \pm 1\rangle\langle n| \otimes |\pm\rangle\langle\pm| = \left[\begin{array}{cc} S_- & 0 \\ 0 & S_+ \end{array} \right] \tag{11}$$

In the last equation, the (1,1) and (2,2) position of the matrix correspond to $|-\rangle\langle-|$ and $|+\rangle\langle+|$, respectively.

Putting it all together, the following unitary matrix serves as the basic discrete time quantum walk operator for one dimensional evolution

$$U = SF_C(\theta). \tag{12}$$

Direct matrix multiplication gives the following standard forms for U:

$$\begin{aligned} U &= \sum_\pm S_\pm \otimes (\sin\theta|\pm\rangle\langle\mp| \mp \cos\theta|\pm\rangle\langle\pm|) && (13) \\ &= \sum_{n=-\infty}^{\infty} \left[\begin{array}{cc} \cos\theta|n-1,-\rangle\langle n,-| & \sin\theta|n-1,-\rangle\langle n,+| \\ \sin\theta|n+1,+\rangle\langle n,-| & -\cos\theta|n+1,+\rangle\langle n,+| \end{array} \right] && (14) \end{aligned}$$

Before introducing arbitrary graphs, we will extend the notation used so far.

[2] We only consider real reflections following Romanelli. See [11] and reference therein for arguments specifying why this is justified.

1.2 Notational reformulation

The notation used so far is how coined quantum walks are usually described. Now we go beyond this by reformulating the notation so that the connection to Szegedy's work becomes more obvious.

If instead of considering the coin space an actual two-dimensional space, we were to consider it as a two-dimensional subspace of the full vertex space then one would probably make the follow identification,

$$|n\rangle|\pm\rangle = |n\rangle|n \pm 1\rangle \tag{15}$$

Notice that nothing is lost or gained since the value of n is encoded in the first space. In this case, $\mathcal{H}_C \subseteq \mathcal{H}_V$ defined relative to each site.

Rewriting (6) using this basis,

$$F^{(n)}(\theta) = \begin{bmatrix} \cos\theta|n-1\rangle\langle n-1| & \sin\theta|n-1\rangle\langle n+1| \\ \sin\theta|n+1\rangle\langle n-1| & -\cos\theta|n+1\rangle\langle n+1| \end{bmatrix}, \tag{16}$$

Unfortunately, the coin-flip operation,

$$F_C = 2\sum |n, f_{n+1,n-1}\rangle\langle n, f_{n+1,n-1}| - \sum |n, n\pm 1\rangle\langle n, n\pm 1| \tag{17}$$

is no longer a reflection on the full vertex space since $|n\rangle\langle n|$ would show up when using $\mathbf{1}\otimes\mathbf{1}$ instead of $\mathbf{1}\otimes\mathbf{1}_\pm$ as in (9). However, we can define a modified identity operator,

$$\mathbf{1}' = \sum |n\rangle\langle n| \otimes |n\pm 1\rangle\langle n\pm 1| \tag{18}$$

such that F_C is again a reflection.

Returning to the shift operator, we rewrite this as

$$S = \sum_{n=-\infty}^{\infty} |n\pm 1, n\pm 2\rangle\langle n, n\pm 1| = \sum_n |n\pm 1\rangle\langle n| \otimes |n\pm 2\rangle\langle n\pm 1| \tag{19}$$

In this space, S is no longer unitary as $SS^\dagger \neq \mathbf{1}\otimes\mathbf{1}$, but is instead equal to the modified identity operator. Note that the relative definition of $|\pm\rangle$ is necessary to give the correct entanglement/correlations between the spaces. This avoids the situation $|n\pm 1\rangle|n\pm 1\rangle$ containing an invalid coin state. This forbids the coin from landing on its "edge" i.e. the state in-between $|n+1\rangle$ and $|n-1\rangle$.

While the notation may seem more cumbersome, it will be useful when trying to generalize to arbitrary graphs and to Szegedy's scheme. In the next section, we will modify the discrete time evolution operator by examining the limitations of the current approach.

1.3 The discrete quantum walk as a product of reflections

The discrete walk on the line has a few special properties that we've been exploiting. First, each vertex of the graph has two neighbors. In a general graph this is not the case and we can circumvent this by considering a larger auxiliary space and reflections on this larger space. As the notation from the previous section should have made clear, the coin space is merely a subspace of the full vertex space spanned by the vertices that are neighbors.

Second, since the walker can shift in more than two directions, the shift operation as defined in (19) is no longer sufficient. Generalizing this to the Szegedy scheme is easiest if we restrict the action of S to the subspace of $\mathcal{H}_V$ spanned by the beginning and ending vertices in both the walker and the auxiliary space. This can be accomplished by changing S such that $n \pm 2$ does appear using an additional operator, $F_x = F_C(\pi/2)$.

$$\sigma = F_x S = \sum |n \pm 1, n\rangle\langle n, n \pm 1| = \sum |n \pm 1\rangle\langle n| \otimes |n\rangle\langle n \pm 1| \tag{20}$$

The shift is still only unitary with respect to the modified identity operator, $S^\dagger F_x^\dagger F_x S = S^\dagger S = \mathbf{1}'$.

Consider two steps of the quantum walks with the new shift operator, σ,

$$\begin{aligned}
(\sigma F_C \sigma) F_C &= \left[\left(\sum_m 2\sigma|m, f_{m+1,m-1}\rangle\langle m, f_{m+1,m-1}|\sigma\right) - \sigma\mathbf{1}'\sigma\right] F_C && (21)\\
&= \left[\left(\sum_m 2|f_{m+1,m-1}, m\rangle\langle f_{m+1,m-1}, m|\right) - \mathbf{1}'\right] F_C && (22)\\
&= \left[2\sum |f_{m+1,m-1}, m\rangle\langle f_{m+1,m-1}, m| - \mathbf{1}'\right] F_C && (23)
\end{aligned}$$

The first term is almost the same as (16) except acting on the left space. Let us relabel $F_C(\theta) = F_R(\theta)$ and define $F_L(\theta) = \sigma F_R(\theta)\sigma$. Now, the two-step quantum walk operator is $F_L(\theta)F_R(\theta)$ which is a product of reflections!

1.4 Generalization to arbitrary graphs

To realize discrete quantum walks on arbitrary graphs, the reflection operators, F_L and F_R, must be generalized. Recalling our work from the previous lectures, the states corresponding to rows of an arbitrary Markov chain P (i.e. $\sum_m P_{nm} = 1$) are

$$|\phi_n\rangle = \sum_m \sqrt{P_{nm}}|n\rangle|m\rangle. \tag{24}$$

The reflection is then defined

$$\begin{aligned}
F_R &= 2\sum_n |\phi_n\rangle\langle\phi_n| - \mathbf{1} && (25)\\
&= \sum_{nmm'} |n\rangle\langle n| \otimes \left(2\sqrt{P_{nm}P_{nm'}} - \delta_{mm'}\right)|m\rangle\langle m'| && (26)
\end{aligned}$$

Note that $\sigma\sigma F_L\sigma = \sigma(\sigma F_L \sigma) = \sigma F_R$. To recover the results of the previous sections, we can use a translational invariant Markov chain, M, defined as follows

$$M_{n,n+1} = \cos^2\omega \tag{27}$$
$$M_{n,n-1} = \sin^2\omega \tag{28}$$
$$M_{n,n\pm1} = M_{n',n'\pm1} \tag{29}$$

One can show that F_R corresponding to Markov chain M the acts on states $|k, k\pm1\rangle$ as (9). Note in (26) we do not use the modified identity operator. The illegal states $|k,k\rangle$ do not evolve under the action of (26) instead only obtaining an alternating phase factor of -1.

The revised shift operator, σ, in (20) swaps the left and right spaces in the walk on a line. Accordingly, we generalize this operator as a swap of the two spaces.

$$\sigma = \sum_{xy} |x,y\rangle\langle y,x|. \tag{30}$$

Finally, we arrive at the generalized discrete time evolution operator for arbitrary graphs

$$\sigma F_R = \sigma\left(2\sum_n |\phi_n\rangle\langle\phi_n| - \mathbf{1}\right) \tag{31}$$

As before, if we consider two-step evolution, then $\sigma F_R \sigma F_R = F_L F_R$ is again a product of reflections. Here we have defined F_L as

$$F_L = \sigma F_R \sigma = \left(2\sum_n |\phi_n\rangle\langle\phi_n| - \mathbf{1}\right) \tag{32}$$
$$= \sum_{nmm'} \left(2\sqrt{P_{nm}P_{nm'}} - \delta_{mm'}\right) |m\rangle\langle m'| \otimes |n\rangle\langle n| \tag{33}$$

In terms of the quantization scheme for pairs of Markov chains Szegedy put forth, we have quantized the Markov chain pair (P, P). To provide further intuition about the Szegedy scheme for discrete time quantum walks, in the next section we discuss the classical analog: a walk on the edges.

2 Intuition from random walks on edges

References [12, 13] nicely describe the idea of a random walk on the edges rather than the vertices. The key idea being that if we use directed edges as the basis for the state space and choose our evolution operators correctly, then we can achieve evolution that matches the vertex based walk. The discussion from this section is summarized in figure 1.

For a walk along the edges, we first specify the state of a walker at a location, l, with a target, t, as $|@l, t\rangle$. The @ is a marker for the origin included for conceptual clarity. Now, consider a tentative transition function, F, based on the transition matrix, P, that has the following action on an edge state:

$$F|@l,t\rangle = \sum_i P_{li}|@l,i\rangle, \tag{34}$$

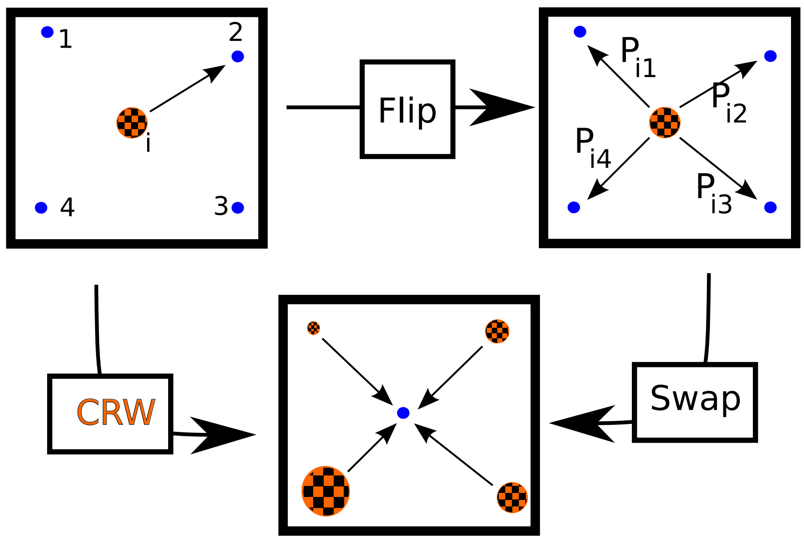


Figure 1: A classical walk on a line using flip and swap operations. The action of the flip operation described in (34) followed by the action of the swap operation in (30). This is the same as a classical walk on the orange check board vertices

for all vertices t. Notice F does not change the origin and only assigns probabilities to the potential moves. This is similar to the flip operator discussed in the quantum case however classically this is not a reflection. To generate motion in the @ space, the proposed moves are acted upon using the same swap operator encountered earlier in the quantum prescription, (30).

If we let $\langle s_0|i\rangle = \sum_j \langle i,j|e_0\rangle$ then for initial vertex state $\langle s_0|$ and initial edge state $|e_0\rangle$, it can be shown that the evolution of $|e_n\rangle = (\sigma F)^n|e_0\rangle$ and $\langle s_n| = \langle s_0|P^n$ are the same after ignoring the second vertex of $|e_n\rangle$. This is left as an exercise for the reader.

To fully compare with the quantum situation, let us remark that the two-step classical walk has a very similar form to the quantum reflective walk. Just as before, we can define alternative transition function F' related to F by $\sigma F\sigma = F'$. Then taking two steps classically, $(\sigma F)^2 = \sigma F\sigma F = F'F$ just as in the quantum case. The relationship between the classical assignment operators F and F' is the same as the relationship between the quantum flip operators, F_L and F_R c.f. (32). The key difference is that the quantum operators are unitary reflection operators while the classical assignment operators are not.

Now we turn to an example recently appearing the in literature: Google in a quantum network by Paparo and Martin-Delgado [9]. For those who have followed the lecture series, the paper should be straightforward to understand and we present here as an example of quantum walks via Markov chain quantization.

3 Google in a quantum network

3.1 The Google matrix

Google's PageRank algorithm is a $25 billion dollar eigenvector problem according to the introductory article [14]. The basic idea of the PageRank algorithm is to mimic a random web surfer (walker) that peruses web pages (vertices) by clicking links at random (edges). The hyperlink matrix is a directed matrix representing the internet. The corresponding Markov chain, E, requires that the weight of each outgoing edge be divided by the number of links on the page so that $\sum_j E_{ij} = 1$. A random walker using transition matrix E is not ergodic because there are some web sites with no outgoing links and some without incoming links. To ensure that the walker doesn't get trapped nor misses any sites, there is a finite probability, α, that the walker will randomly jump to any of the indexed websites. The random jump matrix, C, is such that $C_{ij} = 1/N$ for all i and j. Writing this down as a Markov matrix, G,

$$G = (1 - \alpha)E + \alpha C \tag{35}$$

The PageRank of a website is determined by the stationary distribution, w, of Markov chain G where $wG = w$. The entry w_i corresponding to site i is the importance of site i. The convergence to the stationary distribution, as mentioned in the previous lecture, is determined by the first eigenvalue less than unity, λ_2. For G, eigenvalue depends on α and 0.15 is known to be a reasonable value.

3.2 Quantization

At the end of the last lecture, we showed that the gap $\Delta = 1 - \lambda_2$ is quadratically larger when quantizing reversible Markov chain P and its reversed chain $P^{(*)}$. Thus, quantizing the PageRank algorithm would all the computation of the stationary distribution quadratically faster. However, since the quantum evolution is unitary instead of Markovian, the probability distribution corresponding to a quantum walk never converges to a fixed distribution [6, 8]. However, the time averaged probability does converges.

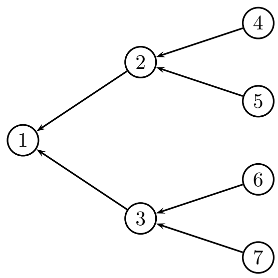
$$\bar{p}(T) = \frac{1}{T}\sum_t p(t) \tag{36}$$

Converting from the quantum wave function, $|\psi\rangle = \sum_{ij} c_{ij}|i\rangle|j\rangle$ to a probability distribution p requires, first, tracing over the second tensor space,

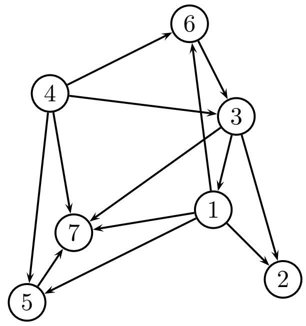
$$\rho^{(1)} = \mathrm{Tr}_2\left(|\psi\rangle\langle\psi|\right) = \sum_j c_{ij}c^*_{i'j}|i\rangle\langle i'|. \tag{37}$$

Second, each diagonal element of $\rho^{(1)}$ are probabilities. That is,

$$p_i = \rho^{(1)}_{ii} = \sum_j |c_{ij}|^2. \tag{38}$$

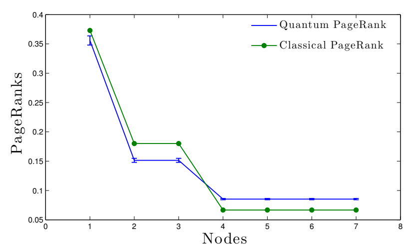


(a) Tree

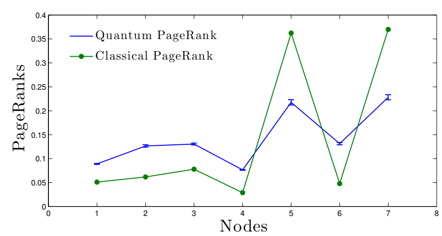


(b) General network

Figure 2: The graphs used to compare the original PageRank algorithm and the quantum PageRank algorithm in [9]. Used with permission.



(a) PageRank for Tree



(b) PageRank for general network

Figure 3: The results of the quantum PageRank algorithm [9] preserve the dominate features and trends of the original PageRank. The error bars on the quantum PageRank points correspond to the variance of the estimate.

The paper by Paparo uses the same quantization scheme discussed in Section 1.4. Additionally, the eigenvalues for the walk are computed following the prescription given in the previous lecture.

Finally, the authors apply the quantized scheme to two small graphs depicted in fig. 2. They compared the time-averaged quantum PageRank and the classical PageRank to find that they differ somewhat as depicted in 3. All figures are used with permission.

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