Quantum speed-up of Markov Chain based algorithms

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Abstract

We develop a generic method for quantizing classical algorithms based on random walks. We show that under certain conditions, the quantum version gives rise to a quadratic speed-up. This is the case, in particular, when the Markov chain is ergodic and its transition matrix is symmetric. This generalizes the celebrated result of Grover [G96] and a number of more recent results, including the element distinctness result of Ambainis [Amb03] and the result of Ambainis, Kempe and Rivosh [AKR] that computes properties of quantum walks on the d-dimensional torus. Among the consequences is a faster search for multiple marked items. We show that the quantum escape time, just like its classical version, depends on the spectral properties of the transition matrix with the marked rows and columns deleted.

1. Hitting Time Based Algorithms

Simulated Annealing, Simulated Evolution (or Genetic Algorithms), and some other individual Monte Carlo algorithms such as Schöning's algorithm [Sch] for a constraint satisfaction problems are stationary stochastic processes on the elements of a finite state space X.

Abstracting out the common mathematical component from the above algorithms we arrive at the following problem: Given a Markov chain with transition probability matrix $P = (p_{x,y})$ on a discrete state space, X, with $|X| = n$ and a subset of marked elements $M \subseteq X$, provide an estimate for the number t of iterations necessary to encounter an element from M for the first time, if we start the chain from a u-distributed element of X. More precisely, we are interested in the expected value of t when u is a given probability distribution on X. To the above hitting time question the answer is well known. Let P_M be the matrix that we obtain from P by deleting its rows and columns indexed from M and let u_M be the vector we obtain from u by deleting entries indexed from M. Let $\mathbf{1}$ be the vector whose all coordinates equal to one. It is not hard to show that the expected value of t is:

$$E(t) = u_M(I - P_M)^{-1}\mathbf{1} \tag{1}$$

If P is irreducible, aperiodic, the matrix $I - P_M$ has an inverse.

A recent breakthrough result of Ambainis [Amb03] and its follow-ups [CE, MSS] have demonstrated that the quantum analogue of random walks can provide fast quantum algorithms not known to be obtainable otherwise. Grover's celebrated search algorithm can also be interpreted as a quantum walk on the edges of a complete graph, and as such it is the first known quadratic speed-up of this kind.

In this paper we work out the analogue of the classical hitting time theory for diffusion based quantum walks. We develop a natural quantization method for ordinary Markov Chains and show that in most cases the quantized walk hits the target set within square root of the classical hitting time. We show that the properties of the walk obtained by quantizing P can be easily computed from the matrix P_M. This creates a bridge between classical and quantum algorithms. We reduce the study of quantum walks to the study of P_M via a simple spectral theorem.

We show furthermore, that the problems of detecting if $M = \emptyset$ and that of finding an $x \in M$ behave differently in the quantum case and that the former is simpler. Much of our study is focused on the case when P is symmetric.

Definition 1 (Spectral Norm) *For a symmetric matrix A let $\lambda(A)$ denote its largest eigenvalue, which is equal to its operator norm,* $\max_{|v|=1} ||Av||$.

The running time analysis of quantum algorithms that detect if $M \neq \emptyset$ depends only on the spectrum of

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P_M, and often only on the spectral norm. The analysis of algorithms that find an element from M requires computing the eigenvectors of P_M as well. Our analysis simplifies many previous results including [Amb03], [AKR] and [SKW]. A preliminary version of part of this article has appeared in [S].

2. Background and Our Results

The notion of quantum walks has emerged gradually, in several steps. The quantum cellular automaton of David Meyer [Mey] made it necessary to understand the behavior of a quantum walks on the one dimensional lattice (line). The next step was made by John Watrous [W] who introduced quantum walks on regular graphs to show that quantum logarithmic space contains classical random logarithmic space. In 2000 Nayak and Vishwanath [NW, ABNVW] gave an explicit form for $|W^t \psi_0 - \psi_0|$, where W is the walk operator of Meyer and ψ_0 is an initial state. Similar questions were studied independently by Aharonov, Ambainis, Kempe and Vazirani [AAKV], and for the mixing time of quantum walks on the circle they gave an almost quadratic bound. They defined the mixing time in terms of a Cezarro limit. They also gave the following general lower bounds:

$$\text{quantum mixing time} \geq \frac{1}{\text{vertex expansion}} \geq \frac{1}{\text{degree} \times \text{conductance}}.$$

This, in particular implies that for a quantum walk on a bounded degree graph the filling, dispersion, sampling and mixing times are at most quadratically better than those of the simple classical random walk on that graph. Hoove and Russel have computed that the mixing time of a quantum walk on the n-dimensional hypercube is n as opposed to the mixing time of the classical walk is only $n \log n$. Kempe computed the hitting time of a walk on the hypercube. Neil Shenvi, Julia Kempe, K. Birgitta Whaley have designed a walk based algorithm to emulate Grover's search [SKW]. The first algorithm in the quantum query model that uses random walks to reduce the number of queries in a search problem and goes beyond Grover is due to Ambainis [Amb03]. He designs a new algorithm for the element distinctness problem which needs only $O(n^{2/3})$ quantum queries. The complexity of his insightful algorithm matches the lower bound of Shi [Sh].

Continuous time quantum walks represent a different line of research. For continuous time parameter t the evolution of these walks is described by the unitary operator e^{itH}, where H is a Hermitian matrix, the so-called Hamiltonian. For quantum walks on edges of a graph G the state space is $\mathbf{C}^{V(G)}$. The Hamiltonian $H = \sum_{v,w \in V(G)} h_{v,w} |v\rangle\langle w|$ has the property that $h_{v,w} \neq 0$ iff $(v,w) \in E(G)$. Continuous time quantum walks were introduced by Farhi and Guttman [FG]. Their power was demonstrated in by A. Childs, E. Farhi, and S. Guttman. [CFG] and even more dramatically by Andrew M. Childs, Richard Cleve, Enrico Deotto, Edward Farhi, Sam Gutmann, Daniel A. Spielman [CCDF]. The papers use a notion of quantum hitting time that is very different from the ours. They prove that the time to go from a distinguished vertex to another one of a certain graph is exponentially faster quantumly than classically. In addition, the [CCDF] paper shows that the speed of quantum algorithm that finds the target vertex is exponentially quicker than any classical (not necessarily walk based) algorithm.

Spatial search problems are search problems with the extra constraint that in a step the algorithm can transfer amplitudes only between "neighboring" states. The neighborhood relation is a binary relation, typically an undirected graph that we shall call *locality structure.* The first study of spatial search was done in [SKW], with the hypercube as locality structure. They showed that the above locality constraint does not add to the running time of Grover search. Subsequently several authors studied the case of the k dimensional torus, $[n]^k$. Aaronson and Ambainis [AaA] gave an almost optimal, $n \log^2 n$, upper bound for $k = 2$. This was a surprise since the torus has very mild expansion properties. Ambainis, Kempe and Rivosh , applying more elegant and more general techniques have achieved a better, $n \log n$ (probably optimal) bound for $k = 2$ and an optimal $n^{k/2}$ upper bound for $k \geq 3$ [AKR]. Childs and Goldstone have considered the same problem from the continuous walk point of view, and in a sequence of improvements they achieved matching results [CG03, CG04]. Our new results generalize [Amb03, AKR] and other quantum search results. The theorems we prove are:

1. For every ergodic Markov chain P with $P = P^T$ the quantum hitting time (appropriately defined) is at most square root of the classical one. This holds for an arbitrary target set $M \subseteq X$.

2. For every ergodic Markov chain P with $P = P^T$, which is also *state transitive* (e.g. it comes from a vertex-transitive graph), and for a single marked element, z, when running the quantized version of P as in 1. we observe z with probability at least $|X|/h$, where h is the average hitting time of the classical version of the chain.

3. Bipartite Walks

Discrete time Markov chains do not naturally quantize. In order to quantize discrete time walks the usual method has been to introduce a coin register in addition to the state register. A walk step is a product of two unitary transformations: The *coin flip* operation acts on the coin register and it is independent of the content of the state register, while the *shift* operation is controlled by the coin register and takes a state to a neighboring state: $|x\rangle|r\rangle \to |x_r\rangle|r\rangle$, where x_r is the r^{th} neighbor of x. The above approach yields quantization easily only of those Markov chains whose transition probabilities are uniform and that are described by d-regular undirected graphs. The coin flip operator changes from literature to literature, but it is most frequently one of the Hadamard or diffusion operators. In this article we propose a quantization that we abstracted out from a recent paper of Ambainis [Amb03] and which is very similar to the quantization model proposed by Watrous in [W]. Our walk model has very advantageous properties: Its two operators are symmetrically defined, it easily encompasses non-uniformity, and the eigenvalues of the walk operator have an elegant mathematical expression. Moreover many current known results easily follow. Among the new consequences are a general search algorithm which detects the presence of several marked items with increased efficiency.

We start with the introduction of bipartite walks in the classical framework remarking that every walk can be made bipartite by a simple "duplicating" operation. Let X and Y be two finite sets and $P = (p_{x,y})$, $Q = (q_{y,x})$ be matrices describing probabilistic maps from X to Y and Y to X, respectively. Since P and Q are stochastic, we have $\sum_{y\in Y} p_{x,y} = 1$ for every $x \in X$ and $\sum_{x\in X} q_{y,x} = 1$ for every $y \in Y$, and all $p_{x,y}$, $q_{y,x}$ are non-negative. If we have a single probabilistic function P from X to X (i.e. a Markov chain), in order to create a bipartite walk we can set $q_{y,x} = p_{y,x}$ for every $x, y \in X$, i.e. we set $Q = P$.

We quantize walk (P, Q) by defining two operators on the Hilbert space with basis states

$$\{|x\rangle|y\rangle \ \mid x \in X, \ \ y \in Y\}.$$

Define states

$$\phi_x = \sum_{y\in Y} \sqrt{p_{x,y}}|x\rangle|y\rangle$$

for every $x \in X$ and

$$\psi_y = \sum_{x\in X} \sqrt{q_{y,x}}|x\rangle|y\rangle$$

for every $y \in Y$. Let $A = (\phi_x)_x$ be the matrix composed of column vectors ϕ_x $(x \in X)$ and $B = (\psi_y)_y$ be the matrix composed of column vectors ψ_y $(y \in Y)$. Our walk operator, W will be the product of

$$\begin{aligned}\text{ref}_1 &= 2AA^* - I;\\ \text{ref}_2 &= 2BB^* - I.\end{aligned}$$

In expression:

$$W = \text{ref}_2\text{ref}_1.$$

Let $\mathcal{C}(A)$ is the column space of A and $\mathcal{C}(B)$ be the column space of B. Observe that $A^*A = I_X$, therefore $(2AA^* - I)A = A$. Also, for any $\phi \in \mathcal{C}(A)^{\perp}$ we have $(2AA^* - I)\phi = -\phi$. Therefore ref_1 is a reflection on the subspace $\mathcal{C}(A)$. Similarly, ref_2 is a reflection on the subspace $\mathcal{C}(B)$. In the study of W a central role will be played by the matrix $D = A^*B$. We call D the discriminant of matrix of the quantized walk operator W. It follows from the definitions that

$$D_{x,y} = \sqrt{p_{x,y}q_{y,x}} \qquad \text{for every } x \in X,\, y \in Y. \qquad (2)$$

Definition 2 (Quantization) *Let P, Q, A, B, D, W as above. Then the quantization of bipartite walk (P, Q) is the unitary operator $W_{P,Q} = W$. We also write $A_{P,Q}$, $B_{P,Q}$ and $D_{P,Q}$ for A, B and D, respectively, if (P, Q) is not clear from the context. If $P = Q$ then we use the shorthand W_P for $W_{P,Q}$, etc.*

4. Spectra of Product of Reflections

Let the columns of matrices A and B be elements of a Hilbert space H and let $A^*A = I_n$, $B^*B = I_m$. Then operators $ref_A = 2AA^* - I$, $ref_B = 2BB^* - I$ are reflections on subspaces $\mathcal{C}(A)$ and $\mathcal{C}(B)$, respectively. In this section we compute spectra of $W = ref_A ref_B$. Our formula turns out to be very useful in the study of quantum walks. Our expressions will use the singular values and vectors of the following matrix:

Definition 3 (Discriminant Matrix) *The* discriminant matrix *for* $\text{ref}_\text{B}\text{ref}_\text{A}$ *is*

$$D(A, B) = A^*B.$$

If we allow the subspaces on which we reflect be represented by arbitrary orthonormed bases (rather than by A and B in particular) then the discriminant matrix is determined only up to unitary multiplicators from left and right.

We can naturally interpret $v \to D(A, B)v$ as a map from $\mathcal{C}(B)$ to $\mathcal{C}(A)$ if we view v as a vector expressed in the $\{b_j\}_{j=1}^m$ bases and the result vector as a one expressed in the $\{a_i\}_{i=1}^n$ bases. To put this into formulas, we can define a map, where Bv is mapped into

$(AA^*)Bv = A\ D(A,B)v$. This map is an orthogonal projection of $\mathcal{C}(B)$ to $\mathcal{C}(A)$, since AA^* is an orthogonal projector to the space $\mathcal{C}(A)$. Similarly $D(A,B)^*$ can be interpreted as an orthogonal projection from $\mathcal{C}(A)$ to the space $\mathcal{C}(B)$. Let λ be a singular value of $D(A,B)$ with associated right singular unit vector v and left singular unit vector w. Then we have

$$\begin{aligned} D(A,B)v &= \lambda w, \\ D(A,B)^*w &= \lambda v. \end{aligned}$$

Since $|Bv| = |v|$, $|Aw| = |w|$, and since projections do not increase length we get:

Lemma 1 *All singular values of $D(A,B)$ are at most one.*

Using the above observation, for a left-right singular vector pair v, w of $D(A,B)$ we can write the associated singular value as $\cos\theta$ for some $0 \leq \theta \leq \frac{\pi}{2}$. In the linear algebra literature θ is called a *canonical angle* between subspaces $\mathcal{C}(A)$ and $\mathcal{C}(B)$. We have that $\theta = 0$ iff the corresponding singular vectors are in $\mathcal{C}(A) \cap \mathcal{C}(B)$. The angle θ has a geometric meaning: it is the angle between Aw and Bv (indeed, $w^*A^*Bv = \cos\theta$).

Theorem 1 (Spectral Lemma) *Let H be a Hilbert space, $A, B \leq H$ subspaces, and let $\mathrm{ref_A}$ and $\mathrm{ref_B}$ be reflections on $\mathcal{C}(A)$ and $\mathcal{C}(B)$. Let $\cos\theta_1, \ldots, \cos\theta_l$ be those singular values of $D(A,B) = A^*B$ that lie in the $(0,1)$ open interval, and let the associated singular vector pairs be v_k, w_k for $(1 \leq k \leq l)$. Then those eigenvalues of the unitary operator $W = \mathrm{ref_B}\mathrm{ref_A}$ that have non-zero imaginary part are exactly*

$$e^{-2i\theta_1},\ e^{2i\theta_1},\ \ldots,\ e^{-2i\theta_l},\ e^{2i\theta_l}. \tag{3}$$

The (un-normalized) eigenvectors associated with these eigenvalues (in order) are

$$\begin{aligned} &Aw_1 - e^{-i\theta_1}Bv_1,\ Aw_1 - e^{i\theta_1}Bv_1,\ \ldots, \\ &\qquad Aw_l - e^{-i\theta_l}Bv_l,\ Aw_l - e^{i\theta_l}Bv_l. \end{aligned}$$

In (3) the singular values are listed with multiplicity. Furthermore,

1. *On $\mathcal{C}(A) \cap \mathcal{C}(B)$ operator W acts as the identity. $\mathcal{C}(A) \cap \mathcal{C}(B)$ coincides with the set of left (right) singular vectors of $D(A,B)$ with singular value 1.*
2. *On $\mathcal{C}(A) \cap \mathcal{C}(B)^\perp$ operator W acts as reflection on the center (i.e. as $-I$). $\mathcal{C}(A) \cap \mathcal{C}(B)^\perp$ coincides with the set of left singular vectors of $D(A,B)$ with singular value 0.*
3. *On $\mathcal{C}(B) \cap \mathcal{C}(A)^\perp$ operator W acts as reflection on the center. $\mathcal{C}(B) \cap \mathcal{C}(A)^\perp$ coincides with the set of right singular vectors of $D(A,B)$ with singular value 0.*
4. *On $\mathcal{C}(A)^\perp \cap \mathcal{C}(B)^\perp$ operator W acts as the identity.*

The above is a complete description of the eigenvalues and eigenvectors of operator W acting on H.

Proof: Let $\pi_A = AA^*$ and $\pi_B = BB^*$ be the orthogonal projector operators (in H) to $\mathcal{C}(A)$ and $\mathcal{C}(B)$, respectively. Then $W = (2\pi_B - I)(2\pi_A - I)$. Since for every v, w singular vector pair with singular value $\cos\theta$ we have $\pi_A Bv = (\cos\theta)Aw$ and $\pi_B Aw = (\cos\theta)Bv$ we can conclude that the (at most) two-dimensional subspace $\langle Bv, Aw\rangle$ is invariant under the action W. Moreover, this action is a composition of two reflections, the first on axis Aw and then on axis Bv. The case when $\langle Bv, Aw\rangle$ is one dimensional gives 1-3, and we leave this easy case to the reader. The subspace $\langle Bv, Aw\rangle$ is two-dimensional if and only if $\cos\theta \in (0,1)$. Considering that the angle between Bv and Aw is θ, the formulas for the spectrum and eigenvalues of W on $\langle Bv, Aw\rangle$ follow from the familiar expressions for the two dimensional case. In particular, it is well known that if we reflect on two axes, we obtain a rotation with an angle that is twice of the one between the axes. Since the set of left and right singular vectors form complete systems, we are done with the description of W on $\langle \mathcal{C}(A), \mathcal{C}B\rangle$. We need to describe W on $\langle \mathcal{C}(A), \mathcal{C}(B)\rangle^\perp = \mathcal{C}(A)^\perp \cap \mathcal{C}(B)^\perp$. On this subspace W is simply a product of two reflections on the center, therefore it is the identity. □

5. The Orbit of a Vector

We keep all notations of the previous section, denote the columns of A by a_i, the columns of B by b_j and define

$$\begin{aligned} \mathcal{C}(A|B) &= \{z \mid\ z = \textstyle\sum c_i a_i + \sum d_j b_j; c_i, d_j \in \mathbf{C}\}. \\ \mathcal{RC}(A|B) &= \{z \mid\ z = \textstyle\sum c_i a_i + \sum d_j b_j; c_i, d_j \in \mathbf{R}\}. \end{aligned}$$

Lemma 2 *Let $D(A,B)$ be real. For $i = 1, 2, \ldots$ let w_i, v_i be the left-right singular vector pairs of $D(A,B)$. Then $z \in \mathcal{RC}(A|B)$ if and only if we can express z as $\sum \nu_i Aw_i + \sum \mu_j Bv_j$, where the coefficients ν_i, μ_j are real.*

Proof: Vectors w_i and v_j have real coefficients and they form complete systems in $\mathbf{C}^m$ and $\mathbf{C}^n$. □

Let $z \in \mathcal{RC}(A|B)$, $|z| = 1$ and let $T > 0$ be an integer for the rest of the section. For a subspace $C \leq \mathcal{C}(A|B)$ let π_C denote the orthogonal projector to C. If C is induced by a single vector h, instead of π_C we write π_h.

For $C \leq \mathcal{C}(A|B)$ we would like to give estimates for the C-component of a typical element of the orbit $z, Wz, W^2z, \ldots, W^Tz$. We define:

$$\mathcal{A}(\pi_C, z, T) = \frac{1}{T+1}\sum_{t=0}^{T} |\pi_C W^t z|^2. \qquad (4)$$

Let $\pi_1, \pi_2, \ldots, \pi_l$ be a complete set of orthogonal projectors ($\pi_i\pi_j = 0$ for $i \neq j$; $\sum \pi_i = I$) and let $C' \leq C$ be subspaces of $\mathcal{C}(A|B)$. Then the following relations are immediate:

$$\begin{aligned} \sum_{i=1}^{l} \mathcal{A}(\pi_i, z, T) &= 1; \qquad (5)\\ \mathcal{A}(\pi_{C'}, z, T) &\leq \mathcal{A}(\pi_C, z, T). \qquad (6) \end{aligned}$$

We first discuss the case, when $C = \langle h \rangle$, where h lies in a two dimensional invariant subspace $\langle Aw, Bv\rangle$, and has real coefficients in terms of Aw and Bv. Let the associated singular value be $\cos\theta$. We will need the identity: $\sum_{t=0}^{t} \cos^2(\alpha + \beta t) =$

$$\frac{1}{2}(T+1) + \frac{\cos(2\alpha + 2T\beta) - \cos(2\alpha + 2(T+1)\beta)}{4(1-\cos 2\beta)} + \frac{\cos 2\alpha - \cos(2\alpha + 2\beta)}{4(1-\cos 2\beta)}. \qquad (7)$$

We may assume that $|h| = 1$ and that the angle between h and z is α. Since W on $\langle Aw, Bv\rangle$ is simply a rotation by 2θ, the projection length of W^tz on h is $\cos(\alpha + 2t\theta)$, so from (7) we get:

$$\mathcal{A}(\pi_h, z, T) = \frac{1}{2} + \frac{\cos(2\alpha + 4T\theta)}{4(T+1)(1-\cos 4\theta)} + \frac{-\cos(2\alpha + 4(T+1)\theta) + \cos 2\alpha - \cos(2\alpha + 4\theta)}{4(T+1)(1-\cos 4\theta)}. \qquad (8)$$

From (8), from inequalities $|\cos\alpha - \cos\beta| \leq |\alpha - \beta|$ and $1 - \cos\alpha \geq \alpha^2/8$ we get:

$$\frac{1}{2} - \frac{1}{(T+1)\theta} \leq \mathcal{A}(\pi_h, z, T) \leq \frac{1}{2} + \frac{1}{(T+1)\theta} \qquad (9)$$

Thus

Lemma 3 *If $T > 10/\theta$, h as above, then $\mathcal{A}(\pi_h, z, T) \geq 0.4$.*

Consider now the more general case, when h is an arbitrary unit vector in $\mathcal{RC}(A|B)$. Let $h = \sum \mu_k h_k$, $z = \sum \nu_k z_k$, where h_k and z_k are unit vectors lying in the invariant subspace $\langle Aw_k, Bv_k\rangle$. We can also assume that ν_k and μ_k are non-negative for every k. Then

$$\mathcal{A}(\pi_h, z, T) = \frac{1}{T+1}\sum_{t=0}^{T}\left(\sum_k \nu_k\mu_k\langle h_k, W^t z_k\rangle\right)^2. \qquad (10)$$

Unfortunately the right hand side of (10) is a trigonometric sum which is not easy to estimate. When C is not one dimensional, our task is even harder. In this case we can proceed by picking an appropriate vector $h \in C$ and reduce the problem to the one dimensional case via inequality (6).

We now start to study another average associated with the orbit of z which will also be useful. Define

$$\mathcal{B}(z, T) = \frac{1}{T+1}\sum_{t=0}^{T}\langle z|W^t z\rangle.$$

We will need the identity

$$\sum_{t=0}^{T} \cos t\beta = \frac{\cos T\beta - \cos(T+1)\beta + 1 - \cos\beta}{2(1-\cos\beta)} \qquad (11)$$

Again, if z lies in invariant subspace $\langle Aw, Bv\rangle$ with associated singular value $cos\theta$, using (11) we get

$$\mathcal{B}(z, T) = \frac{\cos 2T\theta - \cos 2(T+1)\theta + 1 - \cos 2\theta}{2(T+1)(1-\cos 2\theta)}.$$

If $z = \sum \nu_k z_k$ such that z_k (with $|z_k| = 1$) lies in the $\langle Aw_k, Bv_k\rangle$ subspace with associated singular value θ_k then we can express $\mathcal{B}(z, T)$ as

$$\sum_k \nu_k^2 \frac{\cos 2T\theta_k - \cos 2(T+1)\theta_k + 1 - \cos 2\theta_k}{2(T+1)(1-\cos 2\theta_k)}. \qquad (12)$$

The reason that (12) could be expressed in a simpler form than (10) is because in order to obtain (12) we switched the order of the summations over k and T. For (10) we cannot do this because the inside expression is squared. Our goal is to give an *upper* estimate on $\mathcal{B}(z, T)$. Using the trigonometric inequalities as before we get that

$$\mathcal{B}(z, T) \leq \sum_k \nu_k^2 \, \min\{1, \frac{4}{(T+1)\theta_k}\}. \qquad (13)$$

Lemma 4 *Let $E = \sum_k \nu_k^2/\theta_k$, $T \geq 100E$. We have that $\mathcal{B}(z, T) \leq 0.5$.*

Proof: Define $K = \{k \mid \frac{1}{\theta_k} > 10E\}$. We have that $\sum_{k \notin K} \nu_k^2 \leq 0.1$. From this and from (13):

$$\begin{aligned} \mathcal{B}(z, T) \leq \sum_{k \notin K} \nu_k^2 + \sum_{k \in K} \nu_k^2 \frac{4}{(T+1)\theta_k} &\leq \\ 0.1 + \frac{4 \cdot 10E}{100E} &\leq 0.5. \end{aligned}$$

6. Hitting Time, Classical

Let $P = (p_{x,y})$ be the transition matrix of a discrete Markov chain with a finite state space X. The

Markov chain itself is an infinite random walk $x_0, x_1, \ldots$ on states from X, such that $Prob(x_i = y \mid x_{i-1} = x) = p_{x,y}$, independently of states $x_{i-2}, x_{i-3}, \ldots$. One of the most basic concepts of Markov chains is the *hitting time*. For states x and y define $H(x,y)$ as the expected number of steps before state y is visited starting from state x. Hitting times of Markov chains is a very heavily researched area. A Markov chain is *irreducible* if every state is accessible from every other state. For every irreducible Markov chain there is a unique stationary distribution π on the states such that for every $y \in X$

$$\pi_y = \sum_{x \in X} \pi_x p_{x,y}.$$

In other words, $\pi P = \pi$. A Markov chain, by definition, is *reversible* if $\pi_x p_{x,y} = \pi_y p_{y,x}$ for every $x, y \in X$. An irreducible Markov chain is aperiodic if there is a state x and a threshold n_0 such that for every $n > n_0$ the probability that x is reached from x after making exactly n steps is not zero.

Properties of Markov chains are intimately related to the spectrum of their transition matrix. For the *average hitting time* the following nice theorem is known:

Theorem 2 ([BK]) *For an irreducible, aperiodic, reversible Markov chain on n states with transition matrix P we have:*

$$\sum_{x,y \in X} \pi_x \pi_y H(x,y) = \sum_{k=2}^{n} \frac{1}{1-\lambda_k}, \tag{14}$$

Where $1 = \lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$ are the eigenvalues of P.

In [L] we can find an even stronger expression: $\sum_{y \in X} \pi_y H(x,y) = \sum_{k=2}^{n} \frac{1}{1-\lambda_k}$.

7. Searching For Marked Elements, Classical

The algorithmic problem we present below explains our concern with the average hitting time.

Search for Marked: *One or more states in X are marked constituting a set M. Find an element of M.*

Assume we have an initial distribution $\rho = (\rho_x)_{x \in X}$ on the state set X. Starting from a randomly picked element x_0 according to ρ, our machine goes through a sequence of states until it hits an element of M. At every step the probability of transiting from state x to state y is $p_{x,y}$.

Definition 4 *The expected hitting time of M starting from a state x_0 distributed according to ρ is $H(\rho, M) = \sum_{x \in X} \rho_x H(x, M)$.*

Assume that our machine works so that when a marked element is found the machine stays at that state. Thus, it uses a walk operator P' which differs from P on the marked elements. For P' transitions from every marked element $x \in M$ are redefined via $p'_{x,y} = \delta_{x,y}$.

How long do we have to run this machine so that its final state will be with high probability (i.e. with probability greater than 0.5) an element of M? From the Markov inequality it follows that the probability that $x_0 P'^T \notin M$ for $T \geq 2H(\rho, M)$ is less than 0.5. This algorithmic skeleton is used by Schöning [Sch] to improve on the exponent of constraint satisfaction problems.

Definition 5 (The Leaking Walk Matrix) *Let us denote by P_M the matrix that we obtain from P by leaving out all rows and columns indexed by some $x \in M$. If $M = \{x\}$ then we denote P_M by P_x.*

In the rest of the article, unless said otherwise, we assume that P is symmetric ($P = P^T$). This, in particular implies that the stationary distribution is uniform. Let u be the uniform probability distribution on X, and let us denote by $\nu_1, \ldots, \nu_{n-|M|}$ the coefficients of $\hat{u} = \frac{1}{\sqrt{n}} \mathbf{1}_{n-|M|}$ expressed in the basis formed by the normalized eigenvectors of P_M. For the uniform starting distribution Expression (1) takes the form $\frac{1}{n} \sum_{x \in X} H(x, M) = \hat{u}^T (I - P_M)^{-1} \hat{u}$, and if we express the right hand side in the eigen-basis of P_M we get that

$$h_M \stackrel{\text{def}}{=} \frac{1}{n} \sum_{x \in X} H(x, M) = \sum_{k=1}^{n-|M|} |\nu_k|^2 \frac{1}{1-\lambda'_k}, \tag{15}$$

where λ'_k is the k^{th} eigenvalue of P_M.

Definition 6 (Uniform Component) *Let $u = (\frac{1}{\sqrt{d}}, \ldots, \frac{1}{\sqrt{d}})$. The uniform component of a vector $v \in \mathbf{C}^d$ is the u-component of v. Its length is $\langle u \mid v \rangle$.*

Let v be the principal (all-non-negative) eigenvector of P_M, normalized to unit length. In most cases v has a uniform component bounded from below by some constant. From Expression (15) we obtain:

Lemma 5 *If the (normalized) principal (all-non-negative) eigenvector of P_M has a uniform component whose length is bounded from below by a constant then the average hitting of M is in $\Theta\left(\frac{1}{1-\lambda(P_M)}\right)$.*

8. Hitting Time, Quantum

In the rest of the article we use the bipartite walk technique with $X = Y$, $P = P^T$ and $P = Q$. In the previous section we could re-interpret expected hitting time in terms of the modified Markov chain

$$P' = \begin{pmatrix} P_M & P'' \\ 0 & I \end{pmatrix}. \qquad (16)$$

It is easy to show that $\sum_x \pi_x H(x,M)$ roughly coincides with the first t such that $\pi P'^t$ becomes significantly skewed toward M. This happens roughly when the L_1 norm of $\pi P'^t - \pi$ becomes significantly large.

Let W_P be the quantization of P and $W_{P'}$ be the quantization of P' (as in Definition 2). We would like to define the hitting time of W_P with respect to M as the smallest t for which the L_2 norm of $W_{P'}^t \phi_0 - \phi_0$ becomes sufficiently large, where

$$\phi_0 = \frac{1}{\sqrt{n}} \sum_{x,y} \sqrt{p_{x,y}} |x\rangle |y\rangle,$$

a natural starting state, which is invariant under W_P, but at each step slightly changed by $W_{P'}$ until it becomes a very different state. Recall that walk $W_{P'}$ is the quantization of P'. This operator is similar to W_P, but behaves differently on $|x\rangle|y\rangle$ pairs, where $|x\rangle$ or $|y\rangle$ is marked.

Definition 7 *For quantized walk W_P and marked set M we define the hitting time of W_P with respect to target set set M as number of steps, $\mathcal{H}(W_P, M) = T$, for which $\frac{1}{T+1}\sum_{t=0}^{T} |W_{P'}^t \phi_0 - \phi_0|^2$ becomes at least $1 - |M|/|X|$.*

Lemma 6 *Let $v'_1, \ldots, v'_{n-|M|}$ be the normalized eigenvectors of P_M with associated eigenvalues $\lambda'_1, \ldots, \lambda'_{n-|M|}$. For $\hat{u} = \frac{1}{\sqrt{n}}\mathbf{1}_{n-|M|}$ define coefficients $\nu_1, \ldots, \nu_{n-|M|}$ such that $\hat{u} = \sum_{k=1}^{n-|M|} \nu_k v'_k$ holds. Then the hitting time of W_P with respect to M is at most*

$$\frac{100}{1-|M|/|X|} \sum_{k=1}^{n-|M|} \nu_k^2 \sqrt{\frac{1}{1-\lambda_k}}.$$

Proof: By (2) and (16) the discriminant matrix associated with P' is $D = \begin{pmatrix} P_M & 0 \\ 0 & I \end{pmatrix}$. For $1 \le k \le n-|M|$ let v_k be the vector that we obtain from v'_k by augmenting it with zeros on coordinates that are indexed from M. Also, for any $x \in X$ let e_x be the vector that is 1 on x and 0 on all other coordinates. The eigenvectors of D are v'_k $(1 \le k \le n - |M|)$ and e_x $(x \in M)$. For $x \in X$ and a vector v we denote the x coordinate of v by $v[x]$. (Thus $e_x[y] = 1$ iff $x = y$, otherwise $e_x[y] = 0$.) Define

$$\begin{aligned} \phi_k &= \sum_{x \in X} v_k[x] \sqrt{p_{x,y}} |x\rangle|y\rangle \\ \psi_k &= \sum_{x \in X} v_k[y] \sqrt{p_{x,y}} |x\rangle|y\rangle \end{aligned}$$

As a consequence of Theorem 1 we have that for $1 \le k \le n - |M|$ the two-dimensional subspace $S_k = \langle \phi_k, \psi_k \rangle$ is invariant under $W_{P'}$. Let us write $\phi_0 = \phi_{01} + \phi_{02}$, where

$$\begin{aligned} \phi_{01} &= \frac{1}{\sqrt{n}} \sum_{x \in X\setminus M, y \in X} \sqrt{p_{x,y}} |x\rangle|y\rangle; \\ \phi_{02} &= \frac{1}{\sqrt{n}} \sum_{x \in M, y \in X} \sqrt{p_{x,y}} |x\rangle|y\rangle. \end{aligned}$$

Notice that ϕ_{01} and ϕ_{02} are in $\mathcal{RC}(A|B)$. Also:

1. $\langle \phi_{01} \mid \phi_{02} \rangle = 0$;
2. $\langle \phi_{02} \mid \phi_{02} \rangle = p = |M|/|X|$.
3. $\phi_{01} = \sum_{k=1}^{n-|M|} \nu_k \phi_k$.
4. $\langle \phi_{01} \mid \phi_{01} \rangle = 1 - p$, therefore $p + \sum_{k=1}^{n-|M|} \nu_k^2 = 1$.

Set

$$T \ge \frac{100}{1-|M|/|X|} \sum_{k=1}^{n-|M|} \nu_k^2 \sqrt{\frac{1}{1-\lambda_k}} \ge 100 \sum_{k=1}^{n-|M|} \frac{\nu_k^2}{1-p} \theta_k^{-1},$$

arbitrarily. Applying now Lemma 4 for $z = \frac{1}{\sqrt{1-p}}\phi_{01}$ we get that $\mathcal{B}(\phi_{01}, T) \le 0.5$. Thus $\mathcal{B}(\phi_0, T) \le p + (1-p)0.5 = 0.5 + 0.5p$. We need to estimate:

$$\begin{aligned} \frac{1}{T+1} \sum_{t=0}^{T} |W_{P'}^t \phi_0 - \phi_0|^2 &= \\ \frac{1}{T+1} \sum_{t=0}^{T} (2 - 2\langle \phi_0 | W_{P'}^t \phi_0 \rangle) &\ge 1 - p. \quad \square \end{aligned}$$

Corollary 1 *For every ergodic Markov chain such that $P = P^T$, with state space X and for every set $M \subseteq X$, $|M| \le |X|/2$ the hitting time of W_P with respect to M is in the order of the square root of the average hitting time of P with respect to target set M. In formula:*

$$\mathcal{H}(W_P, M) \in O\left(\sqrt{\frac{1}{n} \sum_{x \in X} H(x,M)} \right).$$

Proof: Since $\sum_{k=1}^{n-|M|} \nu_k^2 \le 1$ we have that $\sum_{k=1}^{n-|M|} \nu_k^2 \sqrt{\frac{1}{1-\lambda_k}} \le \sqrt{\sum_{k=1}^{n-|M|} \nu_k^2 \frac{1}{1-\lambda_k}}$. The corollary now follows from Lemma 6 and from (15). $\square$

As an easy corollary of Lemma 6 we also obtain:

Corollary 2 *The hitting time of W_P with respect to any $M \subseteq X$ with $|M| \le |X|/2$ is in $O\left(\sqrt{\frac{1}{1-\lambda(P_M)}}\right)$.*

9. The Detection Problem

In the case of classical walks within the average hitting time, starting from a random element we also find a marked element. For quantum walks the situation is different. Condition $|W_{P'}^t\phi_0 - \phi_0|^2 \geq 1 - |M|/|X|$ does not imply that upon measuring $W_{P'}^t\phi_0$ we get a marked element with constant probability. Often, however, all we need is to solve the following problem:

Detect if Marked: *Let $\mathcal{M} \subseteq 2^X$ be a system of non-empty subsets of M. Given that the set of marked elements is either empty or belongs to $\mathcal{M}$, find out which is the case.*

Lemma 7 *Assume that T is an upper bound for*

$$200 \sum_{k=1}^{n-|M|} \nu_k^2 \sqrt{\frac{1}{1-\lambda_k}},$$

where M runs though all elements of $\mathcal{M}$ (λ_k, ν_k are dependent of M as in Lemma 6). Then we can solve the Detect if Marked problem within time T with bounded one sided error.

Consider the algorithm that receives W, which is either W_P or $W_{P'}$ (does not know which one), randomly picks $1 \leq t \leq T$ and creates the state

$$\frac{1}{2}|0\rangle(\phi_0 + W^t\phi_0) + \frac{1}{2}|1\rangle(\phi_0 - W^t\phi_0), \qquad (17)$$

where the first register above is an additional control register. We measure this state. The content of the $|x\rangle$ register will be a marked element with probability at least $\langle\phi_{02}|\phi_{02}\rangle$. We check if the content of the x register is indeed marked. If yes, we detected marked. If $|M|/|X| \geq 0.5$ this happens with probability at least 0.5. Otherwise we argue: If $W = W_P$ the control register is 0 with probability 1; If $W = W_{P'}$ the control register is 1 with probability at least $\frac{1}{4(T+1)} \sum_{t=0}^{T} |W_{P'}^t\phi_0 - \phi_0|^2 \geq \frac{1}{4}(1 - |M|/|X|)$. Therefore the probability that either a marked element is found in the $|x\rangle$ register or 1 is found in the control register is at least $\frac{1}{8}$.

10. Finding a Marked Element, Quantum

What can be said about finding a marked element instead of detecting if the marked set is non-empty? If the problem has the right structure, we can do a binary search. Often however we need not do binary search because measuring $W_{P'}^t\phi_0$ gives us a marked element with reasonably large probability when t is appropriately set. We will analyze the typical case, when the principal eigenvalue of P_M has a large uniform component. In particular, we show that this is the case if P is symmetric, state-transitive, and $|M| = 1$.

Definition 8 *A Markov chain is state transitive if there is a transitive permutation group acting on the state space that leaves the transition probabilities invariant. In particular, Markov chains created from vertex transitive graphs are state transitive. Throughout this section we denote the eigenvectors of P with $w_1, \ldots, w_n$ with associated eigenvalues $\lambda_1 = 1 > \lambda_2 \geq \lambda_3 \ldots \geq \lambda_n$.*

Lemma 8 *Let $P = (p_{x,y})$ be the transition probability matrix of a symmetric, irreducible, aperiodic, state transitive Markov chain on state space X and let $z \in X$. Then the normalized principal eigenvector of P_z has uniform component of length square at least $\frac{1}{2}$.*

Proof: Let e_x be the characteristic vector of $x \in X$ as before. Fix $z \in X$ (because of the state transitivity it does not matter which one, and later we make a particular choice) and let $e_z = \sum_{k=1}^{n} \delta_k w_k$. Let v be the vector we obtain from the normalized principal eigenvector of P_z by augmenting it with a zero coordinate over z. Let $v = \sum_{k=1}^{n} \nu_k w_k$. Our task is equivalent to proving that $\nu_1^2 \geq 1/2$. If λ is the eigenvalue associated with v, i.e. the spectral norm of P_z, then

$$vP = \lambda v + \nu e_z \qquad (18)$$

for some $\nu \in \mathbf{R}$. From (18), writing down both sides in the $\{w_k\}$ basis, it follows that for $1 \leq k \leq n$:

$$\lambda_k \nu_k = \lambda \nu_k + \nu \delta_k.$$

This implies that for $1 \leq k \leq n$:

$$\nu_k = \frac{\nu \delta_k}{\lambda_k - \lambda}. \qquad (19)$$

Since $\langle v \mid e_z\rangle = 0$, we have that $\sum_{k=1}^{n} \nu_k \overline{\delta_k} = 0$ by $\nu \neq 0$, from which $\sum_{k=1}^{n} \frac{|\delta_k|^2}{\lambda_k - \lambda} = 0$. Therefore

$$\sum_{k=2}^{n} \frac{|\delta_k|^2}{\lambda - \lambda_k} = \frac{|\delta_1|^2}{1-\lambda}, \qquad (20)$$

since $\lambda_1 = 1$. The largest λ that satisfies (20) is between λ_2 and 1, and this is the principal eigenvalue of P_z. Since $\sum_{x \in X} |\langle e_x \mid w_2\rangle|^2 = |w_2|^2 = 1$, there ought to be an $z_0 \in X$ for which $|\langle e_{z_0} \mid w_2\rangle|^2 \geq \frac{1}{n}$. Without loss of generality set $z = z_0$. Then $|\delta_2|^2 = |\langle z_0 \mid w_2\rangle|^2 \geq \frac{1}{n}$. Since $|\delta_1|^2 = \frac{1}{n}$, we get from (20) that $\frac{1}{\lambda - \lambda_2} \leq \frac{1}{1-\lambda}$. From this $1 - \lambda \leq \lambda - \lambda_2$ implying $1 - \lambda \leq \lambda - \lambda_k$ for every $2 \leq k \leq n$. Using this, from (20) we get that

$$\sum_{k=2}^{n} \frac{|\delta_k|^2}{(\lambda - \lambda_k)^2} \leq \frac{|\delta_1|^2}{(1-\lambda)^2}.$$

which implies $\sum_{k=2}^{n} \nu_k^2 \le \nu_1^2$, and since $\sum_{k=1}^{n} \nu_k^2 = 1$, we get that $\nu_1^2 \ge 1/2$, what we needed. $\square$

Theorem 3 *Let $M = \{z\}$. Let $W_{P'}$ be the quantization of P' above and let $T \ge 10\sqrt{\frac{1}{1-\lambda(P_z)}}$. Then the probability that for a randomly chosen $t \in [1, T]$ we observe z in the second register when measuring $W_{P'}^t \phi_0$ is $\Omega(n(1-\lambda))$.*

Proof: Consider the quantized walk, P', with $M = \{z\}$. Let v be as in Lemma 8, and define

$$\phi = \frac{1}{\sqrt{n}} \sum_{x,y} v[x] \sqrt{p_{x,y}} |x\rangle |y\rangle; \tag{21}$$

$$\psi = \frac{1}{\sqrt{n}} \sum_{x,y} v[y] \sqrt{p_{y,x}} |x\rangle |y\rangle. \tag{22}$$

The two-dimensional space $S = \langle \phi, \psi \rangle$ is invariant under $W_{P'}$. Indeed, write down the discriminator matrix for $W_{P'}$: $D = \begin{pmatrix} P_z & 0 \\ 0 & 1 \end{pmatrix}$ and notice that v is an eigenvector of D. Then use Theorem 1. Lemma 8 implies that ϕ_0 has a ϕ component of length square at least $1/2$. We study $W_{P'}^t \phi$ and show that it will have a large z component. Notice that $W_{P'}$ turns ϕ in the invariant subspace S, and after roughly $t = \frac{\pi}{2\theta}$ steps, where $\theta = \arccos\langle \phi | \psi \rangle$, the resulting vector, $W_{P'}^t \phi$, becomes roughly parallel with $\phi - \psi$. Define $h = (\phi - \psi)/|\phi - \psi|$. We show:

Lemma 9 *The squared Z component of h is at least $n(1-\lambda)/8$, where $Z = \langle \sum_{x \in X} \alpha_x |x\rangle |z\rangle \mid \alpha_x \in \mathbf{C} \rangle$.*

Proof: we have:

$$|\phi - \psi|^2 = 2(1 - \cos\theta) = 2(1 - \lambda). \tag{23}$$

The squared Z component of $\phi - \psi$ is

$$\sum_{x \in X} v[x]^2 p_{x,z}.$$

From the analysis of Lemma 8, using (19) with $k = 1$ and noting that $\lambda_1 = 1$, $\delta_1 = \frac{1}{\sqrt{n}}$ and $|\nu_1| \ge 1/2$ we obtain:

$$|\nu| \ge \sqrt{n}(1 - \lambda)/2 \tag{24}$$

Since $\nu = \sum_{x \in X} v[x] p_{x,z}$, we obtain

$$\sum_{x \in X} v[x]^2 p_{x,z} \ge \left(\sum_{x \in X} v[x] p_{x,z} \right)^2 = \nu^2 \ge n(1 - \lambda)^2 / 4.$$

From (23) and from the above we get that the squared Z component of h is at least

$$\frac{n(1-\lambda)^2}{8(1-\lambda)} = n(1-\lambda)/8. \qquad \square$$

We need to show that this large Z component of $W_{P'}^t \phi$ implies a large Z component of $W_{P'}^t \phi_0$. This is almost apparent, since the squared ϕ component of ϕ_0 is at least 0.5, but the subtle point that no cancellation occurs is left for the full version. $\square$

Remark 1 $\Omega(1 - \lambda) = \Omega(1/h)$, *where h is the average hitting time of chain P with respect to $M = \{z\}$. Because of the state transitivity we can just talk about average hitting time.*

Corollary 3 *In Theorem 3 we can replace the lower bound formula for the probability of observing z by the formula $\Omega(n/h)$, where h is the average hitting time of the classical walk with transition probability matrix P.*

11. Consequences

The theorems tie together the theory of symmetric classical and quantum walks. We obtain two-ways connections for both the hitting time and the observation probabilities when the chain is state-transitive. The classical results for the $[n]^d$ torus are summarized below [AF]:

Dimension	Average Hitting Time
1	n^2;
2	$n^2 \log n$;
$d \ge 3$	n^d;

We "quantize" the above table. We replace h with $\sqrt{h}$ and setting n/h for the observation probabilities in all rows we get that in the quantum case:

Dimension	Hitting Time	Observation probability
1	n	$1/n$;
2	$n\sqrt{\log n}$	$\frac{1}{\log n;}$
$d \ge 3$	$n^{d/2}$	$\Omega(1)$.

In fact, for any Cayley graphs(regardless if Abelian or not) we can use known classical bounds to obtain properties of the corresponding quantum walks. There are also several methods in store to estimate the spectral norm of P_M, when $M > 1$. For instance

Lemma 10 *Let the spectral gap of P be at least δ and $|M|/n \ge \varepsilon$ then $\lambda(P_M) \le 1 - \varepsilon\delta/2$*

From this lemma and from known results on Johnson graphs the analysis of the walk in [Amb03] is immediate.

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