Almost uniform sampling via quantum walks

Peter C. Richter*

Abstract

Many classical randomized algorithms (e.g., approximation algorithms for \#P-complete problems) utilize the following random walk algorithm for almost uniform sampling from a state space $S$ of cardinality $N$: run a symmetric ergodic Markov chain $P$ on $S$ for long enough to obtain a random state from within $\epsilon$ total variation distance of the uniform distribution over $S$. The running time of this algorithm, the so-called mixing time of $P$, is $O(\delta^{-1}(\log N + \log \epsilon^{-1}))$, where $\delta$ is the spectral gap of $P$.

We present a natural quantum version of this algorithm based on repeated measurements of the quantum walk $U_t = e^{-iPt}$. We show that it samples almost uniformly from $S$ with logarithmic dependence on $\epsilon^{-1}$ just as the classical walk $P$ does; previously, no such quantum walk algorithm was known. We then outline a framework for analyzing its running time and formulate two plausible conjectures which together would imply that it runs in time $O(\delta^{-1/2} \log N \log \epsilon^{-1})$. We prove each of the conjectures for the standard walk on a restricted class of graphs: the torus $\mathbb{Z}_p^d$, $p$ prime, and the hypercube $\mathbb{Z}_2^n$.

1 Introduction

1.1 Quantum walks and algorithms

In the design of quantum algorithms, we are interested in identifying problems whose time complexity appears to drop significantly if we allow solution by a quantum computer. Notable examples discovered thus far include the hidden subgroup problem (Simon [35], Shor [34], Kitaev [27], Hallgren [20]) and the unstructured search problem (Grover [19]). While the apparent quantum speedup is exponential for the hidden subgroup algorithms (which use the powerful quantum Fourier transform), the quadratic speedup of Grover’s search algorithm is significant in that it is transferrable to a broad array of problems, as the search problem is perhaps the most fundamental in computer science.

Over the last several years, a family of algorithms based on quantum walks (see the surveys by Kempe [23] and Ambainis [5]) has emerged as a considerable generalization of Grover’s algorithm. A quantum walk is the analogue of a classical random walk in that it is the powering of a single, often sparse, matrix; in the quantum case this matrix is unitary rather than stochastic. Discrete-time quantum walks were first investigated in the computer science community by Meyer [30] and Watrous [38], then more explicitly by Nayak et al. [32] and Aharonov et al. [1]. They have been used in quantum algorithms for the element distinctness problem (Ambainis [4]), matrix product verification (Burhman and Spalek [8]), finding triangles in graphs (Magniez, Santha, and Szegedy [29]), finding subsets (Childs and Eisenberg [11]), and group commutativity testing (Magniez and
Nayak [28]). Continuous-time quantum walks were introduced by Childs, Farhi, and Gutmann [17, 12]. They were used by Childs et al. [10] to solve in polynomial time an oracle problem for which no polynomial-time classical algorithm exists.1

1.2 Quantum hitting and mixing times

Each of the quantum walk algorithms we have just mentioned solves a particular instance of the following abstract search problem: given a graph structure (i.e., a state space with allowed transitions) and a subset of states which are marked, find a marked state (if one exists) by performing a quantum walk on the graph. In the decision version of the problem, we need only detect with constant success probability whether or not the marked subset is nonempty; we call its complexity (measured in walk steps) the quantum hitting time.2 The discrete- and continuous-time versions of the quantum hitting time on various graphs have been studied by a number of researchers (see e.g., [4, 24, 33, 7, 13, 14, 9]). Szegedy [36, 37] extended the notion of discrete-time quantum hitting time to “quantized” Markov chains and showed the following general result: given a symmetric ergodic Markov chain with classical hitting time \( \tau_{\text{hit}} \), we can define a natural unitary quantum walk with the same locality whose quantum hitting time is \( O(\tau_{\text{hit}}^{1/2}) \). In particular, the classical hitting time of a Markov chain with spectral gap \( \delta \) and a fraction \( \varepsilon \) of its states marked is \( O((\delta \varepsilon)^{-1}) \), so the quantum hitting time is \( O((\delta \varepsilon)^{-1/2}) \).

For classical Markov chains, the mixing time parameter is as significant in applications as the hitting time, if not more so. The mixing time of an ergodic Markov chain measures the time past which the current state distribution is within \( \varepsilon \) distance of its (limiting) stationary distribution over all states, independent of what the initial state was. Thus, the mixing time characterizes the complexity of sampling from the states of a Markov chain with respect to the stationary distribution. The most famous application in theoretical computer science is in the Markov chain Monte Carlo (MCMC) method for approximate sampling and counting. An important special case is the problem of almost uniform sampling (see Jerrum [21]), where we wish to output an element from within \( \varepsilon \) total variation distance of the uniform distribution over a finite set, in this case by running a symmetric Markov chain whose stationary distribution is uniform over the set until it has \( \varepsilon \)-mixed.

1.3 Our contributions

In light of the success of quantum walks in speeding up classical search algorithms, an obvious question to ask is: can classical sampling algorithms based on mixing of random walks be sped up by using quantum walks instead? Aharonov et al. [1] were the first to look closely at the subject of (time-averaged) limiting distribution for a quantum walk and to define a notion of quantum mixing time to reach this distribution. A number of important questions were raised in their paper. We consider two in particular, the first being: which distributions can we generate using quantum walks? Aharonov et al. [1] showed that the limiting distribution of the quantum walk on a regular graph is typically non-uniform (and even dependent on the initial state); we give a simple algorithm based on repeated measurements of the continuous-time quantum walk \( U_t = e^{-itP} \) for a symmetric ergodic Markov chain \( P \) (inspired by the decohering quantum walk of Kendon and

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1Continuous-time quantum walks can be simulated efficiently by (discrete-time) quantum circuits using techniques which we discuss in Section [5].

2The search and decision versions for classical random walks have the same complexity; this does not appear to be true for quantum walks.
Tregenna [24, 25] that necessarily outputs a state $\epsilon$-close to the uniform distribution. Moreover, it does so with only logarithmic dependence on $\epsilon^{-1}$, just as the classical walk $P$ does.

The second question of Aharonov et al. [1] that we consider is: when does quantum mixing offer a speedup over classical mixing? This question seems to be a great deal more difficult than the first (e.g., Aharonov et al. [1] only demonstrated a quantum speedup for the discrete-time walk on a cycle); we provide a framework for answering this question and then formulate two strong but plausible conjectures that, if true, would solve it: (a) that threshold quantum mixing can be achieved in $O(\delta^{-1/2} \log N)$ time, and (b) that amplification to $\epsilon$-mixing from threshold-mixing can be achieved in $O(\log \epsilon^{-1})$ time (independent of $N$). In particular, if both conjectures are true, then there is an $O(\delta^{-1/2} \log N \log \epsilon^{-1})$ quantum algorithm for almost uniform sampling, as opposed to the $O(\delta^{-1}(\log N + \log \epsilon^{-1}))$ classical algorithm. We prove the amplification conjecture for the standard walk on the torus $\mathbb{Z}_p^n$, $p$ prime (the proof is more subtle than one might expect), and we prove the threshold mixing conjecture for the hypercube $\mathbb{Z}_2^n$. It is our hope that our approach and progress on the problem of almost uniform sampling via quantum walks will rejuvenate interest in characterizing the speedup of quantum mixing.

2 Preliminaries

2.1 Classical and quantum processes

Let $S$ be a set of states with $|S| = N$. Consider the $N$-dimensional complex vector space $\mathcal{H}(S)$ with basis states $\mathcal{B}(S) := \{|s\} : s \in S\}$; in particular, this space contains the pure quantum states (i.e., wavefunctions) $\mathcal{W}(S) := \{ |\phi\rangle = \sum_{s \in S} \phi_s |s\rangle : \phi_s \in \mathbb{C}, \forall s \in S, ||\phi||_2 = 1\}$. It also contains the classical randomized states (i.e., distributions) $\mathcal{D}(S) := \{ p = \sum_{s \in S} \phi_s |s\rangle : p_s \in \mathbb{R}_0, \forall s \in S, ||p||_1 = 1\}$.

For our purposes, it will suffice to consider the three following physically realizable processes: stochastic evolution $\mathcal{D}(S) \rightarrow \mathcal{D}(S)$ (e.g., a symmetric Markov chain $P$), unitary evolution $\mathcal{H}(S) \rightarrow \mathcal{H}(S)$ (e.g., the quantum walk $U_t : |\phi\rangle \mapsto e^{-iPt}|\phi\rangle$), and the projective measurement $\mathcal{H}(S) \rightarrow \mathcal{D}(S) : |\phi\rangle \mapsto \sum_{s \in S} |s\rangle\langle s|\phi\rangle$.

Remark. Processes with quantum operations and intermediate measurements produce mixed states (i.e., randomized ensembles of quantum states) and are typically described by their action on density matrices; however, our algorithm and its analysis are more simply described using classical and quantum state vectors alone.

2.2 Basic properties of Markov chains

The long-term behavior of a discrete-time Markov chain $P$ and its continuous-time counterpart (Poisson average) $\exp(-(I-P)t) = \sum_{s=0}^{\infty} e^{-t}\lambda^s P^s$ is summarized by the following theorems.

Theorem 2.1 (Unique stationary distribution) Let $P$ be irreducible (i.e., strongly connected). Then there exists a unique stationary distribution $\pi$ for $P$.

In particular, if $P$ is symmetric then the uniform distribution $u := \left(\frac{1}{N}, \ldots, \frac{1}{N}\right)^\dagger = \frac{1}{N} 1^\dagger$ is stationary.\footnote{Note that the “missing” process $\mathcal{D}(S) \rightarrow \mathcal{H}(S)$ is unnecessary, since it can be described as the linear combination of its (non-interfering) actions on basis states $\mathcal{B}(S)$, which are a special case of unitary evolution.}

Throughout this paper, we use the term Markov chain when describing either the actual chain ($\{P^t\}$ in discrete time, $\{\exp(-(I-P)t)\}$ in continuous time) or the stochastic matrix $P$ generating the chain.

\footnote{We use $1^\dagger$ to denote the $N$-dimensional column vector of ones; $\dagger$ is the conjugate transpose.}

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An irreducible Markov chain $P$ converges in the Cesaro (i.e., time-averaged) and continuous-time (i.e., Poisson-averaged) limits to its stationary distribution:

**Theorem 2.2 (Fundamental theorem)** Let $P$ be irreducible. Then the stochastic matrices $\frac{1}{T} \sum_{t=0}^{T-1} P^t$ and $\sum_{s=0}^{\infty} e^{-t}\frac{1}{s!} P^s$ tend to $[\pi \pi \cdots \pi] = \pi 1^\dagger$ as $T \to \infty$. If $P$ is also aperiodic (i.e., non-bipartite), then $P^t \to \pi 1^\dagger$ as $t \to \infty$, and we call $P$ ergodic.

An irreducible Markov chain is reversible if it satisfies the detailed balance constraints $P_{ij}\pi_j = P_{ji}\pi_i$; or equivalently, if the matrix $S = DPD^{-1}$ is symmetric, where $D$ is the diagonal matrix with $D_{ii} = \sqrt{\pi_i}$. The spectral gap $\delta$ of a Markov chain $P$ is the difference between its largest and second-largest eigenvalues. The mixing time $\tau(\epsilon)$ of an ergodic discrete-time Markov chain is $\min\{T : \frac{1}{2}||P^t - \pi 1^\dagger||_1 \leq \epsilon \forall t \geq T\}$, where $\frac{1}{2}|| \cdot ||_1$ is the total variation distance.

**Theorem 2.3 (Diaconis, Strook [16]; Aldous [2])** Let $P$ be reversible and ergodic. Then its mixing time satisfies $\frac{1}{2} \lambda \delta^{-1} \ln(2\epsilon)^{-1} \leq \tau(\epsilon) \leq \delta^{-1}(\ln \pi_{\text{min}}^{-1} + \ln \epsilon^{-1})$, where $\pi_{\text{min}} := \min_x \pi(x)$.

The mixing time of any irreducible Markov chain $P$ can be defined using the Cesaro average, the Poisson average, or the lazy chain $\frac{1}{2}(I + P)$; in each case, the mixing time behaves similarly up to the dependence on $\epsilon$. In most applications the key factor in Theorem 2.3 is the spectral gap. Sometimes we can compute this directly; other times we estimate it, say via conductance (see e.g., [22, 21]).

Theorem 2.3 implies that the following single-loop classical mixing algorithm samples from a distribution $\epsilon$-close to $\pi$ for any ergodic $P$, from any initial state:

**Algorithm 2.4 (Single-loop classical)** Do $\tau(\epsilon)$ times: Apply $P$ to the current state.

In describing our quantum algorithm for almost uniform sampling, we will appeal to the notions of threshold mixing and amplification, which are implicit in the classical Markov chain mixing algorithm as well. In particular, a (slightly weaker) variant of the previous theorem follows from combining the next two well-known theorems:

The threshold mixing time $\tau_{\text{mix}}$ of an irreducible Markov chain is $\tau_{\text{mix}} := \tau(1/2\epsilon)$.

**Theorem 2.5 (Amplification)** For any Markov chain $P$, $\tau(\epsilon) \leq \tau_{\text{mix}}[\ln \epsilon^{-1}]$.

**Theorem 2.6 (Threshold mixing - Aldous [2])** Let $P$ be reversible and ergodic. Then $\delta^{-1} \leq \tau_{\text{mix}} \leq \delta^{-1}(1 + \frac{1}{2} \log \pi_{\text{min}}^{-1})$.

In light of the amplification and threshold mixing theorems, we can view the same classical mixing algorithm as a double-loop algorithm instead: the inner loop builds the fast-mixing threshold matrix $P^{\tau_{\text{mix}}}$ from $P$, and the outer loop iterates this matrix only $[\ln \epsilon^{-1}]$ times to achieve $\epsilon$-mixing.

**Algorithm 2.7 (Double-loop classical)** Do $[\ln \epsilon^{-1}]$ times: { Do $\tau_{\text{mix}}$ times: Apply $P$ to the current state. }

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6 We have implicitly assumed here that the second-largest eigenvalue of $P$ exceeds the smallest in absolute value; this is easy enough to arrange in practice by replacing $P$ with $\frac{1}{2}(I + P)$.  

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2.3 Additional properties of Markov chains

We will use several more facts about Markov chains and their mixing properties beyond the basic ones already mentioned; we present them here with proofs for completeness.

Why do we set the threshold mixing time $\tau_{\text{mix}}$ to $\tau(1/2e)$? We do it precisely so that the amplification theorem holds (i.e., so that $P^\tau_{\text{mix}}$ $\epsilon$-mixes in time $O(\log \epsilon^{-1})$). It so happens that the choice $1/2e$ is rather arbitrary beyond the fact that it is a fixed constant below $1/2$, as the following generalization of the amplification theorem shows.

**Proposition 2.8** Let $Q$ be a Markov chain with maximum pairwise column distance $\max_{x,x'} \frac{1}{2} ||Q(\cdot,x) - Q(\cdot,x')||_1 \leq \alpha < 1$. Then it has mixing time $\tau(\epsilon) \leq \lceil \log_{1/\alpha}/\epsilon \rceil$.

**Proof:** From Aldous and Fill [3]: Let $\bar{d}(t)$ := $\max_{x,x'} \frac{1}{2} ||Q^t(\cdot,x) - Q^t(\cdot,x')||_1$ be the maximum pairwise column distance at time $t$. This distance is submultiplicative; i.e., $\bar{d}(s+t) \leq \bar{d}(s)d(t)$ for any $s, t \geq 0$. In particular, $\bar{d}(t) \leq \bar{d}(1)^t$, so $\bar{d}(\lceil \log_{1/\alpha}/\epsilon \rceil) \leq \epsilon$, where $d(t) := \frac{1}{2} ||Q^t - \pi^1||_1$ and $\pi$ is the stationary distribution of $Q$.

In particular, if $T \geq \tau(1/2e)$, then the columns of $P^T$ are $(1/2e)$-close to their common limit $\pi$, so they have maximum pairwise distance at most $1/e$. It follows that $P^T$ mixes in time $\lceil \log_{e}/\epsilon \rceil = \lceil \ln e^{-1} \rceil$, yielding the amplification theorem.

So in order to show that a Markov chain mixes in time $O(\log \epsilon^{-1})$, it suffices to show that its columns have maximum pairwise distance at most some constant less than one. A sufficient condition for this property to hold is the following:

**Proposition 2.9** Let $\beta > \frac{1}{2}$, $\gamma > 0$; let $Q$ be an $N \times N$ stochastic matrix with at least $\beta N$ entries in each column bounded below by $\gamma/N$. Then $\max_{x,x'} \frac{1}{2} ||Q(\cdot,x) - Q(\cdot,x')||_1 \leq 1 - \gamma(1 - 2(1 - \beta)) < 1$.

**Proof:** Recall that for any two distributions $p,q$ we have $\frac{1}{2} ||p - q||_1 = 1 - \sum_k \min\{p_k, q_k\}$. It follows that $\max_{x,x'} \frac{1}{2} ||Q(\cdot,x) - Q(\cdot,x')||_1 \leq 1 - (1 - 2(1 - \beta))N \cdot \gamma/N = 1 - \gamma(1 - 2(1 - \beta))$.

We can estimate the maximum pairwise distance of a Markov chain $Q'$ from that of a nearby chain $Q$ using the triangle inequality:

**Proposition 2.10** Let $Q$ and $Q'$ be Markov chains; let $\beta := \frac{1}{2} ||Q - Q'||_1$ and $\gamma := \max_{x,x'} \frac{1}{2} ||Q(\cdot,x) - Q(\cdot,x')||_1$. Then $\max_{x,x'} \frac{1}{2} ||Q'(\cdot,x) - Q'(\cdot,x')||_1 \leq 2\beta + \gamma$.

**Proof:** For any $x, x'$: $\frac{1}{2} ||Q'(\cdot,x) - Q'(\cdot,x')||_1 \leq \frac{1}{2} ||Q'(\cdot,x) - Q(\cdot,x)||_1 + \frac{1}{2} ||Q'(\cdot,x') - Q(\cdot,x')||_1$.

3 A quantum algorithm for almost uniform sampling

3.1 A single-loop algorithm

Let $P$ be an irreducible reversible Markov chain with uniform stationary distribution on the set $S$ of states; equivalently, $P$ is an irreducible symmetric Markov chain. We wish to sample almost uniformly from $S$ using the quantum walk $U_t = \exp(-iPt)$ (i.e., $P$ is the time-independent Hamiltonian, or complex Hermitian matrix, driving the walk) from any initial basis state $|x\rangle \in B(S)$. Aharonov et al. [1] propose (a discrete-time version of) the following “single-loop” algorithm:
Algorithm 3.1 (Single-loop quantum) Run the walk \( U = e^{-iPt} \) for time \( t \) chosen uniformly at random (u.a.r.) from \([0,T]\), then measure and output the current state.

Let \( P_t(y,x) := \langle y|e^{-iPt}|x\rangle^2 \) be the stochastic matrix mapping inputs to outputs for this algorithm for a fixed \( t \); then the finite-time Cesaro matrix \( \bar{P}_T := \frac{1}{T} \int_0^T P_t \, dt \) maps inputs to outputs for \( t \) chosen u.a.r. from \([0,T]\). Unlike \( P_t \) (whose columns oscillate as \( t \to \infty \)), \( \bar{P}_T \) has a limit \( \Pi \) as \( T \to \infty \), which we call the infinite-time Cesaro matrix. This is demonstrated by the following continuous-time version of Theorem 3.4 from Aharonov et al. \( \Pi \), which also gives an upper bound on the quantum mixing time \( \tau'(\epsilon) := \min\{T' : \frac{3}{2}||\bar{P}_T - \Pi||_1 \leq \epsilon \forall T \geq T'\}:

Theorem 3.2 (Cesaro matrices) Let \( H \) be a Hamiltonian with spectrum \( \{\lambda_k,|\phi_k\rangle\} \). Let \( \{C_j\} \) be the partition of these indices \( k \) obtained by grouping together the \( k \) with identical \( \lambda_k \). Then:

\[
\bar{P}_T(y,x) = \sum_j \left| \sum_{k \in C_j} \langle \phi_k|x\rangle \langle \phi_k|\phi_k\rangle \right|^2 + \sum_{k,l : \lambda_k \neq \lambda_l} \langle \phi_k|x\rangle \langle \phi_k|\phi_l\rangle \langle \phi_l|\phi_k\rangle \langle \phi_l|y\rangle \frac{1}{T} \int_0^T e^{i(\lambda_k - \lambda_l) t} \, dt
\]

As \( T \to \infty \) the latter term tends to zero, so the limit \( \Pi \) of \( \bar{P}_T \) exists and is equal to the former term. Hence the quantum mixing time \( \tau'(\epsilon) \) is the smallest \( T' \) such that for all \( T \geq T' \) we have:

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\frac{1}{2}||\bar{P}_T - \Pi||_1 = \max_x \sum_y \left| \sum_{k,l : \lambda_k \neq \lambda_l} \langle \phi_k|x\rangle \langle \phi_k|\phi_l\rangle \langle \phi_l|\phi_k\rangle \langle \phi_l|y\rangle \frac{1}{T} \int_0^T e^{i(\lambda_k - \lambda_l)t} \, dt \right| \leq \epsilon
\]

It can be inferred from this theorem that both the discrete- and continuous-time walks typically lack the property \( \Pi = u1^\dagger = \frac{1}{N} \times \) the all-ones matrix (which we require to mix to uniform, or even to mix to the same distribution from any two initial states, using the above algorithm), except in special circumstances such as when the walk takes place on the Cayley graph of an Abelian group and it has distinct eigenvalues. It so happens that these two special properties hold for the discrete-time walk on the cycle (with Hadamard coin flip); Aharonov et al. \( \Pi \) show this and then use Theorem 6.2 to prove that \( \tau'(\epsilon) \leq O(N \log N \epsilon^{-2}) \) for this walk, yielding a quantum algorithm for almost uniform sampling on the cycle that is nearly quadratically faster than the classical simple random walk. They further show that walks with the property \( \Pi = u1^\dagger \) can be sequentially repeated in such a way that the distance of the output state from uniform drops exponentially with the number of walk repetitions (i.e., the dependence on \( \epsilon^{-1} \) is logarithmic), just like it does for classical Markov chains. In particular, this reduces the time required to sample almost uniformly from the cycle to \( O(N \log N \log \epsilon^{-1}) \).

3.2 A double-loop algorithm

What about the (typical) case when \( \Pi \neq u1^\dagger \)?\(^7\) Then not only is it unclear how to obtain the exponential drop in closeness to uniform (i.e., logarithmic dependence on \( \epsilon^{-1} \)), but the single-loop algorithm does not even sample almost uniformly, but rather from a non-uniform distribution dependent on the initial state. To remedy this, we propose the following “double-loop” algorithm:

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\(^7\)For a walk on the symmetric group \( S_n \), Gerhardt and Watrous \( 13 \) showed that \( \frac{1}{2}||\Pi - u1^\dagger||_1 \geq \frac{1}{2} - \frac{1}{n!(n-1)}^{2n-2} \); for a walk on the hypercube \( Z_2^n \), Moore and Russell \( 31 \) showed that there exists an \( \epsilon > 0 \) such that \( \frac{1}{2}||\Pi - u1^\dagger||_1 \geq \epsilon. \)
Algorithm 3.3 (Double-loop quantum) Do $T'$ times: Run the walk $U = e^{-iPt}$ for time $t$ chosen u.a.r. from $[0, T]$, then measure and output the current state.

This is almost the same algorithm proposed by Aharanov et al. $\Pi$ to obtain logarithmic dependence on $\epsilon^{-1}$ in the special case $\Pi = u1^\dagger$, but we claim that for any $\Pi$ our algorithm: (a) samples almost uniformly, and (b) does so with logarithmic dependence on $\epsilon^{-1}$.

Let’s prove claim (a):

**Theorem 3.4 (Uniform mixing)** If $P$ is a symmetric irreducible Markov chain, then each entry of $\Pi$ is bounded from below by $1/N^2$; in particular, $\Pi$ is ergodic. Moreover, each of the $P_t$ (and so $\Pi_t$ and $\Pi$ as well) is symmetric and therefore has uniform stationary distribution.\(^8\)

**Proof:** The 1-eigenspace of $P$ is precisely the space spanned by $u$, so it follows from Theorem 1.2 that $\Pi(y,x) \geq 1/N^2$ for every $x, y$. To see that $P_t(y,x) := |\langle y | e^{-iPt} | x \rangle|^2$ is symmetric, write out the Taylor series for $e^{-iPt}$ and note that every positive integer power $P^k$ is symmetric (since $P^2(x,y) = \sum_z P(x,z) \cdot P(z,y) = \sum_z P(y,z) \cdot P(z,x) = P^2(y,x)$). It follows that the stationary distribution of $P_t$ is uniform.\(^9\)

This implies that for any $\epsilon > 0$ our algorithm will (for $T$ and $T'$ sufficiently large) output a state $\epsilon$-close to uniform, so claim (a) is proven.

Now let’s prove claim (b), and in the process obtain upper bounds on the minimum $T$ and $T'$ required for our algorithm to output a state $\epsilon$-close to uniform. First a few definitions: For a particular quantum walk $e^{-iPt}$, fix $\alpha := \max_{x,x'} \frac{1}{2} \| \Pi(y,x) - \Pi(y,x') \|_1$. We define the quantum threshold mixing time of the walk to be $\tau_{\text{mix}}' := \tau'(\epsilon_0)$, where (for the time being) we set $\epsilon_0 := \frac{1}{T^2}$. Then we have the following easy theorem:

**Theorem 3.5 (Convergence time)** For $T = \tau_{\text{mix}}'$ and $T' = \lceil \log_2/(1+\alpha) \epsilon^{-1} \rceil$, our algorithm outputs a state $\epsilon$-close to uniform.

**Proof:** For any $T \geq \tau_{\text{mix}}'$, the Markov chain $\bar{P}_T$ built by the inner loop is $\epsilon_0$-close to its limit $\Pi$, where $\epsilon_0 = \frac{1}{T^2}$. By definition, the maximum pairwise column distance of $\Pi$ is at most $\alpha$. So by Proposition 2.10 $\bar{P}_T$ has maximum pairwise column distance at most $2\epsilon_0 + \alpha = \frac{1+\alpha}{2}$. Since the outer loop is a $T'$-fold repetition of $\bar{P}_T$, choosing $T' \geq \lceil \log_2/(1+\alpha) \epsilon^{-1} \rceil$ yields an output state within $\epsilon$ distance of uniform by Proposition 2.8.

We can now state clearly what we hope to be able to do: run the quantum walk (inner loop) for a long enough time $T$ so that the matrix $\bar{P}_T$ is within a small (but still constant) threshold distance $\epsilon_0$ from its limit $\Pi$, at which point it must have maximum pairwise column distance less than some constant below one (provided that $\Pi$ itself has this property) and therefore need only be applied $T' = O(\log \epsilon^{-1})$ times (independent of $N$) to output a state $\epsilon$-close to uniform. In particular, this motivates us to make the next two strong but plausible conjectures for the quantum walk $U_t = e^{-iPt}$ for symmetric irreducible $P$:

**Conjecture 3.6 (Amplification)** The supremum $\alpha_0$ of $\alpha$ over all such quantum walks is strictly less than one.

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\(^8\) $\Pi$ is also positive semidefinite: it is the Gram matrix of $\{f_s\}$ with $f_s(kl) := \langle s| \phi_k \rangle \langle \phi_l | s \rangle$ if $\lambda_k = \lambda_l$, 0 otherwise.

\(^9\) More generally, the uniform distribution is stationary for any process consisting of unitary evolution followed by measurement, since it is invariant under both operations.
This would imply that we can always choose $T' = O(\log \epsilon^{-1})$. Of course, this matters little unless the quantum threshold mixing time is significantly faster than the classical threshold mixing time; to this end, we conjecture:

**Conjecture 3.7 (Threshold mixing)** Any such quantum walk satisfies $\tau_{mix}' \leq O(\delta^{-1/2} \log N)$.

This would imply that we can always choose $T = O(\delta^{-1/2} \log N)$. It would also imply (by Cheeger’s inequality) that the threshold quantum mixing time is $\tilde{O}(1/\Phi)$ where $\Phi$ is the conductance of $P$, a question posed by Aharonov et al. [1]. By Theorem 3.5, the validity of both conjectures would give us an $O(\delta^{-1/2} \log N \log \epsilon^{-1})$ quantum algorithm for almost uniform sampling.

### 4 Proving the amplification and threshold mixing conjectures

#### 4.1 Intuition

To show that the amplification conjecture holds for a particular $P$, we need an upper bound on the maximum pairwise column distance of $\Pi$. One way to do this is via Proposition 2.9, which tells us that it suffices to show that most of the entries in each column of $\Pi$ are $\Omega(1/N)$. We can view this as a statement that the quantum walk is ergodic in a weak sense; i.e., that from any initial basis state, the limit of the time-averaged distribution over states induced by the quantum walk is roughly equivalent to the space-averaged (uniform) distribution. Indeed, for Proposition 2.9 not to hold, almost all of the mass from the time-averaged quantum walk distribution must be localized over a minority of the states. Using Theorem 3.2, we have already shown a lower bound of $1/N^2$ on each entry of $\Pi$ (Theorem 3.1). More detailed knowledge of the spectrum of $P$ allows us to tighten this lower bound, as we shall soon see in the case of the walk on the torus.

To show that the threshold mixing conjecture holds for a particular $P$, we need to know how fast the quantum walk propagates. It is known that the distribution induced by a quantum walk spreads quadratically faster than the corresponding random walk distribution on the line and on higher-dimensional lattices, for example; on the other hand, it cannot spread asymptotically faster than the (already optimally-spreading) random walk distribution on a bounded-degree expander. Our conjecture is motivated by these two observations, and is supported by the fact that $O(\delta^{-1/2} \log N)$ is a known upper bound on the diameter of a regular graph. In particular, it is true for the (discrete-time) quantum walk on the cycle (Aharonov et al. [1]) and for the quantum walk on the hypercube, which we will discuss shortly.

#### 4.2 The torus $\mathbb{Z}_p^d$

We prove the amplification conjecture for the $d$-dimensional torus $\mathbb{Z}_p^d$, $p$ prime. The next two lemmas were proven with the help of Mario Szegedy.

**Lemma 4.1 (Eigenvalue multiplicities of $\mathbb{Z}_p^d$)** Let $P$ be the standard transition matrix on $\mathbb{Z}_p^d$ with $d \geq 1$ fixed, $p > 4d$ prime, and $N = p^d$. Then each of the $C_j$ consists of all $l \in \mathbb{Z}_p^d$ equivalent to a single $k \in \mathbb{Z}_p^d$ up to permutation and signing of the coordinates.

**Proof:** Let $\omega = e^{2\pi i/p}$. Suppose $\lambda_k = \lambda_l$ and $l$ is not equivalent to $k$. Then the vanishing sum

$$
\sum_{j=1}^{d} \omega^{kj} + \omega^{-kj} - \omega^{lj} - \omega^{-lj} = 0
$$

(4)
is not simply 2d vanishing sums of length two $\omega^{kj} - \omega^{-kj}$ over $j : 1 \leq j \leq d$. Observe that if we cannot decompose the above sum into length-two vanishing sums in precisely this way, then we cannot do so at all (since $\omega^{kj} + \alpha = 0 \Rightarrow \alpha = -\omega^{kj}$ is a 2pth root of unity but not a pth root of unity). Hence there exists a minimal vanishing sum of length $m$ ($3 \leq m \leq 4d$) of roots of unity $\zeta_j$ (wlog, wma $\zeta_1 = 1$) of common order $r = p$. By Theorem 5 of Conway and Jones [15], $\sum_{s \text{ prime}: s \mid r} (s - 2) \leq m - 2$; so we have $p - 2 \leq 4d - 2$.

Lemma 4.2 (Eigenvector cancellations for $Z^n_d$) For any $y \in Z^n_d$, there are $\Omega(n)$ different $x \in Z_n$ satisfying $xy_i \mod n \in [-n/8d, n/8d]$ for all $i : 1 \leq i \leq d$.

Proof: Consider the map $f : Z_n \to Z^n_d$ given by $x \mapsto (xy_1, \ldots, xy_d)$. Thinking of $Z^n_d$ as being divided into subgrids of side length $n/m$ (with one of them, $H_0$, centered at 0), it is clear that one such subgrid (call it $H$) must contain at least $n/m^d$ of the points in the image of $f$. Let $x'y$ be any of the image points in $H$. Then there are at least $n/m^d$ different $x$ for which $(x - x')y_i \in [-n/m, n/m]$ for all $i$. Let $m = 8d$; then there are at least $n/(8d)^d$ such $x$.

Theorem 4.3 (Amplification for $Z^n_d$) Let $P$ be the standard transition matrix on $Z^n_d$ with $d \geq 1$ fixed, $p$ prime, and $N = p^d$. Then each entry of $\Pi$ is bounded below by $\Omega(1/N)$, so the amplification conjecture is satisfied.

Proof: Label the spectrum of $P$ using indices $k \in Z^n_d$ as follows:

$$\lambda_k := \frac{1}{d} \sum_{j=1}^{d} \cos(2\pi ik_j/p) \quad \phi_k := \frac{1}{\sqrt{N}} \sum_{x \in Z^n_d} e^{2\pi ik \cdot x/p} |x|$$

(5)

Since $Z^n_d$ is vertex-transitive, it suffices to show that $\Pi(y,0) = \Omega(1/N)$; or, from Theorem 5.2

$$\sum_j \left| \sum_{k \in C_j} e^{2\pi ik \cdot y/p} \right|^2 = \Omega(N)$$

(6)

This is a consequence of the preceding two lemmas: by Lemma 4.2 at least $(p/(8d)^d)^d = \Omega(N)$ of the $k \in Z^n_d$ are such that: (i) $k \cdot y_i \mod p \in [-p/8d, p/8d]$ \forall i, j, thus (ii) $l \cdot y := \sum_i l_i y_i \mod p \in [-p/8, p/8]$ for all $l$ equivalent to $k$ up to permutation and signing of the coordinates. So by Lemma 4.1, which in particular shows that $|C_j| \leq 2^d d!$ for all $j$, it follows that $(p/(8d)^d)^d/2^d d! = \Omega(N)$ of the $C_j$ give a sum of at least 1.

4.3 The hypercube $Z^n_2$

We now give a simple argument showing that the threshold mixing conjecture holds for the hypercube $Z^n_2$. The first observation is well-known (e.g., see Moore and Russell [31]):

Lemma 4.4 (Periodicity for $Z^n_2$) Let $P$ be the standard transition matrix on $Z^n_2$, and let $|\psi_t\rangle$ be the wavefunction induced by the quantum walk $U_t = e^{-iPt}$. Then $|\psi_{2\pi n+t}\rangle = |\psi_t\rangle$ for all $t$.

Proof: The eigenvalues of $P$ are $1 - 2|k|/n$ for $k \in Z^n_2$, where $|\cdot|$ is the Hamming weight. So the eigenvalues of $U_{2\pi n+t}$ are all equal to one; i.e., $U_{2\pi n}$ is the identity.
Theorem 4.5 (Threshold mixing for $\mathbb{Z}_2^n$) Let $P$ be the standard transition matrix on $\mathbb{Z}_2^n$. Then $\tau'_{\text{mix}} \leq O(n)$, so the threshold mixing conjecture is satisfied.

Proof: Let $T = q \cdot 2\pi n + r$, where $q \in \mathbb{Z}$ and $0 \leq r < 2\pi n$. Then by the triangle inequality, we have

$$\frac{1}{2}||\bar{P}_T - \Pi||_1 \leq q \cdot \frac{1}{2} ||\bar{P}_{2\pi n} - \Pi||_1 + \frac{1}{2} ||\bar{P}_r - \Pi||_1 \leq \frac{r}{T},$$

since $\bar{P}_{2\pi n} = \Pi$ (by Lemma 4.4). Hence, $\frac{1}{2}||\bar{P}_T - \Pi||_1 \leq \epsilon_0$ for all $T \geq \frac{2\pi n}{\epsilon_0}$. \hfill \blacksquare

5 Simulability and applications

5.1 Simulation by quantum circuits

The quantum walk $U_t = e^{-iPt}$ is the continuous-time evolution of a time-independent Hamiltonian. This is a valid model of quantum computation; however, the discrete-time quantum circuit model is often preferred due to its similarity to the classical digital circuit model. We can simulate the continuous-time quantum walk (and our algorithm) in the circuit model in one of two ways: either by replacing the walk by its discrete-time counterpart (in which case simulability is immediate), or by showing that the dynamics of the walk are well-approximated (i.e., $||U_t - U||_2 \leq \epsilon$) by a small quantum circuit $U$.\footnote{On the other hand, the classical continuous-time random walk for time $t$ is trivial to simulate: simply run the corresponding discrete-time random walk for $s$ steps, where $s$ is the Poisson random variable with parameter $t$.}

We describe briefly how to do the latter; for more detail, see Childs [9].

Let $H$ be a Hamiltonian and $\sum_{j=1}^r H_j$ be a decomposition of $H$ into Hamiltonians $H_j$. We can simulate $H$ by evolving the $H_j$ one at a time (in round-robin fashion) by the Lie product formula

$$e^{-iHt} = (e^{-iH_1t/2} \cdots e^{-iH_rt/2})^j + O(\max_{k,l} ||[H_k, H_l]||_2 r t^2 / j)$$

(8)

where $[A, B]$ is the commutator $AB - BA$. Of course, we then have to worry about simulating each of the $H_j$, but this should be rather straightforward assuming that we have chosen a good decomposition $\sum_{j=1}^r H_j$. For example, if $H = P$ is the standard transition matrix for the Cayley graph of an Abelian group (product of $d$ cyclic groups), then we consider the natural 2d-coloring of the edges $E = \cup_{j=1}^{2d} E_j$ (alternate between two colors along each of the $d$ directions) and choose each $H_j = P_j$ ($1 \leq j \leq r = 2d$) such that $P_j(x,y) = P(x,y)$ for all $(x,y) \in E_j$ and $P_j(x,y) = 0$ for all $(x,y) \notin E_j$. Then each of the $[P_k, P_l]$ is zero and each of the $P_j$ is the disjoint union of locally simulable interactions, so the overall simulation yields no asymptotic loss in efficiency.

5.2 Application to the MCMC method

In the design of a fully-polynomial randomized approximation scheme (FPRAS) for a $\#P$-complete problem (e.g., the permanent of a matrix $[22]$), it is often sufficient to construct a fully-polynomial almost uniform sampler (FPAUS) over the set of witnesses (solutions) $\mathbb{Z}_2$. Markov chain Monte Carlo (MCMC) algorithms do this by performing a random walk over the set of witnesses. The mixing time of this walk shows up in the running time of the FPRAS; in fact, proving that the walk is rapidly mixing is typically the most challenging aspect of designing an FPRAS. If our quantum walk algorithm can be shown to offer a speedup over the classical random walk, it could potentially yield quantum speedups for a number of FPRAS’s.
6 Conclusions and open problems

We have presented for the first time a natural quantum algorithm based on the quantum walk $U_t = e^{-iPt}$ that samples from a distribution $\epsilon$-close to uniform with logarithmic dependence on $\epsilon^{-1}$ for any symmetric irreducible Markov chain $P$. We have outlined a framework for analyzing its running time and formulated two plausible conjectures which together would imply that it runs in time $O(\delta^{-1/2} \log N \log \epsilon^{-1})$. We have proven each of the conjectures for the standard walk on a restricted class of graphs: the torus $\mathbb{Z}_p^d$, $p$ prime, and the hypercube $\mathbb{Z}_2^n$.

The most important problems we have left open are the resolution of the amplification and threshold mixing conjectures. We note that the conjectures can be worked on independently, and that partial progress (as we have obtained for $\mathbb{Z}_p^d$ and $\mathbb{Z}_2^n$) is indeed possible. In particular, we would like to see the threshold mixing conjecture proven for $\mathbb{Z}_p^d$ or the amplification conjecture proven for $\mathbb{Z}_2^n$, so that the running time of our algorithm is determined for either $\mathbb{Z}_p^d$ or $\mathbb{Z}_2^n$. Also, we believe that it should be possible to prove the amplification conjecture for $\mathbb{Z}_n^d$, $n$ composite or $d = \omega(1)$, by extending our line of argument.

Another question is whether the decohering walk of Kendon and Tregenna [26] (which is similar to our algorithm, only with Poisson-distributed rather than regular Cesaro-distributed walk measurements) solves the almost uniform sampling problem with roughly the same running time as our algorithm; we suspect the answer is yes. Perhaps it can even be analyzed more easily than our algorithm for certain classes of walks.

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