

A Model of Coinless Quantum Walks and Quantum Markov Chain Monte Carlo

Gillian Grindstaff, Kevin Wilson*

Advisor: Yevgeniy Kovchegov

Oregon State University

August 16, 2013

Abstract

We consider a transformation that will produce a unitary matrix from a stochastic matrix, in particular matrices implemented in Markov chain Monte Carlo methods, as a means of defining a quantum dynamical system which will converge on a desired probability distribution. For the uniform cyclic walk on n states, we give a full characterization of the quantum operator which will produce the uniform vector.

1 Introduction

Recently there has been considerable research in quantum algorithms modeling random walks on graphs and Markov chains. Szegedy[10] discussed applications of results in graph theory and MCMC methods to Grover's algorithm[9] and others. Dimcovic[3] discussed a framework for modeling quantum walks which utilized a separate coin space and state space to determine the action of the walk. This work was continued in previous REU projects at Oregon State University. In this paper we discuss a method of modeling random walks with Markov chains in a quantum system without the use of a coin space. We take a stochastic matrix forming the basis of a dynamical Markov chain system and directly transform it into a unitary Hermitian operator for an analogous quantum dynamical system which acts in a similar way.

*Funding was provided by the National Science Foundation through the REU program at Oregon State University

In Section 2 we discuss necessary quantum background information, including an introduction to Hilbert spaces, quantum algorithms, and quantum operators. In Section 3 we reintroduce the Metropolis-Hastings Algorithm[11][12] in the context of quantum computation, and in Section 4 we provide a complete algorithmic process for the transformation of a stochastic matrix. In Section 5, optimize the algorithm in a specific case by bypassing a matrix inversion for the uniform walk on the n -cycle, and in the final Section 6, we examine questions of algorithmic locality and future research.

2 Background

To start, let us begin with a few necessary definitions when discussing quantum computation.

Definition 1. *Given an n -dimensional Hilbert space \mathcal{H}_n a quantum state $|\psi\rangle$ is a superposition of basis states $|0\rangle, \dots, |n-1\rangle$, in the form $|\psi\rangle = \sum_{j=0}^{n-1} \alpha_j |j\rangle$ such that $\sum_{j=0}^{n-1} |\alpha_j|^2 = 1$.*

The values $|\alpha_j|^2$ represent the probability that after measurement that state $|j\rangle$ appears as the post-measurement state.

Definition 2. *Operator U is **unitary** if $U^*U = UU^* = I$. This implies U preserves lengths of input vectors, is normal, and thus has an orthonormal basis of eigenvectors of \mathcal{H}_n with eigenvalues $\{e^{i\theta_1}, \dots, e^{i\theta_n}\}$.*

Definition 3. *Operator H is **hermitian** if $H = H^*$. This implies H is normal, and thus has an orthonormal basis of eigenvectors of \mathcal{H}_n with real eigenvalues $\{\lambda_1, \dots, \lambda_n\}$.*

Schrodinger's equation,

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

determines the evolution of a quantum system based on a hermitian operator H , called the Hamiltonian of the system. Solving this system shows that a unitary operator dictates the discrete transition from one state to another. Thus, we must use a unitary operator $U_{n \times n}$ when acting on n -qubit quantum states. For example, basic examples of single qubit operations of quantum states in a 2-dimensional Hilbert space \mathcal{H}_2 include the Pauli matrices and the Hadamard matrix, as listed below:

$$\text{Pauli } X : X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\text{Pauli } Y : Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\text{Pauli } Z : Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\text{Hadamard} : H = \frac{|0\rangle + |1\rangle}{\sqrt{2}}\langle 0| + \frac{|0\rangle - |1\rangle}{\sqrt{2}}\langle 1| = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$$

Of frequent use in our project is the Quantum Fourier Transform (QFT). Given a superposition of states $|\psi\rangle = \sum_{j=0}^{N-1} x_j |j\rangle$, the n -dimensional QFT, denoted F_n , maps it to the following:

$$F_N(|\psi\rangle) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} y_k |k\rangle, \text{ where } y_k = \sum_{j=0}^{N-1} x_j \omega^{jk}, \text{ and } \omega = e^{2\pi i/N}$$

$$F_N = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \dots & \omega^{(N-1)^2} \end{pmatrix}$$

Using tools such as these, one can create quantum algorithms designed for operation on a quantum computer. Examples include Shor's factorization algorithm, Grover's algorithm, and phase estimation.

Quantum walks, an application of quantum operations, represent the quantum analog of the classical random walk, in which a manipulation of quantum states in an n -dimensional Hilbert space \mathcal{H}_n occurs over a unitary operator acting in a similar manner as a stochastic operator in classical random walks. In our paper, we look to construct a quantum analog for the Metropolis-Hastings algorithm in MCMC (Markov Chain Monte Carlo) operations, specific to the case where one constructs the uniform stationary distribution. This work is in preparation for further work in constructing an arbitrary stationary distribution, such as the Metropolis-Hastings algorithm accomplishes.

3 Markov Chain Monte Carlo Methods

3.1 Metropolis-Hastings Algorithm

In the classical Metropolis-Hastings algorithm, we begin with a given probability distribution π , and construct a Markov chain that imitates a system converging on π .

Let Q be any column stochastic transition matrix, called a **proposal** transition matrix, and let $a_{ij} = \min(1, \frac{\pi(j)Q_{ij}}{\pi(i)Q_{ji}})$ for $i \neq j, Q_{ji} \neq 0$. We simulate a walk that exhibits the following behavior:

1. Begin at a random vertex x_t for $t = 0$.
2. Randomly pick x'
3. Accept x' with probability $a_{x_t x'}$. If accepted, let $x_{t+1} = x'$. If not, $x_{t+1} = x_t$.
4. Continue to pick x' , accept or reject, until the desired sample size is obtained.

We can do this with a Markov chain system based on the following transition matrix:

$$P_{ij} = \begin{cases} Q_{ji}a_{ij} & \text{if } i \neq j \\ 1 - \sum_{j \neq i} P_{ij} & \text{if } i = j \end{cases}$$

I.e. given an arbitrary initial vector ψ_0 , $P^T \psi_0$ approximates π . For the purposes of this paper we use the shorthand $P = MH(\pi, Q)$ to indicate the matrix produced by the Metropolis-Hastings method, using ratios of $\pi(i)/\pi(j)$ and entries of Q to construct a_{ij} and the matrix entries as defined above.

Remark 1. *We note the following facts about the transformation $P = MH(\pi, Q)$:*

1. $P = MH(\pi, Q)$ is always reversible.
2. If $i \neq j$ and $Q_{ij} = 0$, then $P_{ij} = P_{ji} = 0$.

We intend to transform the Metropolis-Hastings probability matrix P into a unitary matrix U , for implementation in a quantum computer. We consider various choices for Q that might simplify the procedure, and determine computability and rates of convergence.

3.2 Quantum Implementation

Following the Metropolis-Hastings Algorithm, we suppose we have some matrix G of dimension n and probability distribution π , also of dimension n . Let

$$a_{ij} = \min \left(1, \frac{\pi(j)G_{ij}}{\pi(i)G_{ji}} \right),$$

and create the matrix P_{ij} as described. We apply the diagonal matrices $D^{1/2}$ and $D^{-1/2}$ from section 2.2. Simplifying this procedure, we can bypass construction and symmetrization and directly define P' as the following:

$$P'_{ij} = \min \left(\frac{\sqrt{\pi(i)}}{\sqrt{\pi(j)}} g_{ji}, \frac{\sqrt{\pi(j)}}{\sqrt{\pi(i)}} g_{ij} \right)$$

$$P'_{ii} = 1 - \sum_{j \neq i} \min \left(g_{ji}, g_{ij} \frac{\pi(j)}{\pi(i)} \right)$$

And we apply the abovementioned transformation W :

$$U = e^{i\theta} (P' - \alpha I) (P' - \bar{\alpha} I)^{-1}$$

This yields a unitary matrix, and the extraction method described in Section 2.3 will yield a vector with distribution $\xi_0 \sqrt{\pi}$ in the first n qubits, where ξ_0 is the inner product of the input vector with $\sqrt{\pi}$.

3.2.1 Specific Example

Note that in the Metropolis-Hastings algorithm, we have free choice of matrix Q . In this paper, however, we concentrate on modeling the simple walk on a discrete cycle of length n , thus for this algorithm we use the specific example of $Q = G$ as shown below.

$$G = \begin{pmatrix} 0 & 1/2 & 0 & \dots & 1/2 \\ 1/2 & 0 & 1/2 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 1/2 & 0 & 1/2 \\ 1/2 & \dots & 0 & 1/2 & 0 \end{pmatrix}$$

$$g_{ij} = \begin{cases} 1/2 & \text{if } |i - j| = 1 \pmod n \\ 0 & \text{otherwise} \end{cases}$$

Thus we can simplify the formulation of P' from the previous section.

$$P'_{ij} = \begin{cases} \frac{1}{2} \min \left(\frac{\sqrt{\pi(i)}}{\sqrt{\pi(j)}}, \frac{\sqrt{\pi(j)}}{\sqrt{\pi(i)}} \right) & \text{if } |i - j| = 1 \pmod n \\ 1 - \frac{1}{2} \left(\min(1, \frac{\pi(i-1)}{\pi(i)}) + \min(1, \frac{\pi(i+1)}{\pi(i)}) \right) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

For $\pi = (\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n})$, we show an explicit form for U in Equation 5.9.

4 Algorithm

4.1 Random Walks on a Graph

Here we reimagine the following classical random walk: we have N nodes $0, 1, 2, \dots, N-1$, such that node k is adjacent to node $k-1$ and $k+1$. A particle starting at 0 moves

to 1 or $N - 1$ with probability $\frac{1}{2}$. Classically, we model this dynamical system with a Markov chain, with the following matrix:

$$P = \begin{pmatrix} 0 & 1/2 & 0 & \dots & 1/2 \\ 1/2 & 0 & 1/2 & \dots & 0 \\ 0 & 1/2 & 0 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1/2 & 0 & \dots & 1/2 & 0 \end{pmatrix} \quad (4.1)$$

We consider this matrix as a function on N -dimensional vector space, with vector ψ_t representing a probability distribution over the nodes at time t . It is acted upon discretely by P , i.e. $\psi_t = P^t \psi_0$, where ψ_0 is the initial position, and t is the number of steps completed. We first note that the spectrum of this P , a circulant matrix, is given by

$$\lambda_j = \frac{1}{2}\omega_j + \frac{1}{2}\omega_j^{n-1}, \quad j = 0 \dots n - 1.$$

where $\omega_j = e^{\frac{2\pi i j}{n}}$ is a complex n^{th} root of unity. Note that $\lambda_0 = 1$ is the largest eigenvalue. The eigenvectors of this bad boy are always corresponding columns of the discrete Fourier transform.[5]

From well-known results in stochastic processes, any ergodic P has a stationary or equilibrium distribution π such that $P\pi = \pi$, i.e. π is an eigenvector of P corresponding to eigenvalue 1.

4.2 Unitary Matrix U

In order to find a quantum algorithm for evaluation of steady-state problems, we translate this process into an analogous chain of unitary matrices, which will act on n -dimensional vectors in Hilbert space \mathcal{H} in a similar manner to P . Suppose π is a probability distribution on n vertices. We show that 1 is an eigenvalue of U , with corresponding eigenvector $\sqrt{\pi} = (\sqrt{\pi(1)}, \sqrt{\pi(2)}, \dots, \sqrt{\pi(n)})$, as H is equipped with \mathcal{L}_2 , rather than \mathcal{L}_1 norm.

To construct U , we first define the symmetric matrix P' which is similar to P :

$$P' = DPD^{-1}$$

where D is the diagonal matrix with $D(i, j) = \delta_{ij}\sqrt{\pi(i)}$.

Remark 2. *The symmetry of P' is dependent on the reversibility of P : note that $P'_{ij} = \sqrt{\pi(i)}P_{ij}(\sqrt{\pi(j)})^{-1}$. If P is reversible, $\pi(i)P_{ij} = \pi(j)P_{ji}$, and thus several algebraic manipulations give us $P'_{ji} = P'_{ij}$.*

We define θ and α such that

$$e^{i\theta} \frac{1 - \alpha}{1 - \bar{\alpha}} = 1$$

and we construct U in the following manner.

$$U = e^{i\theta} (P' - \alpha I)(P' - \bar{\alpha} I)^{-1}. \quad (4.2)$$

Remark 3. U is, in fact, unitary: since P' is real and symmetric and αI is diagonal, $(P' - \alpha I)^* = P' - \bar{\alpha} I$, and thus $U^* = e^{-i\theta} (P' - \alpha I)^{-1} (P' - \bar{\alpha} I)$. Therefore, when multiplying U and U^* together, we see

$$U^*U = (P' - \alpha I)^{-1} (P' - \bar{\alpha} I) (P' - \alpha I) (P' - \bar{\alpha} I)^{-1}$$

Since $P' - \alpha I$ and $P' - \bar{\alpha} I$ have the same eigenspaces, they commute. Continuing through our sequence of equations,

$$U^*U = (P' - \alpha I)^{-1} (P' - \alpha I) (P' - \bar{\alpha} I) (P' - \bar{\alpha} I)^{-1} = I$$

Remark 4. Furthermore, U has an eigenvalue of 1, and thus a corresponding stationary eigenvector $\sqrt{\pi}$.

If we represent $P' = QSQ^{-1}$, where S is the diagonal matrix of eigenvalues of P' and the columns of Q are eigenvectors of P' , we see that

$$U = e^{i\theta} (QSQ^{-1} - \alpha I)(QSQ^{-1} - \bar{\alpha} I)^{-1}$$

$$U = e^{i\theta} Q(S - \alpha I)Q^{-1}Q(S - \bar{\alpha} I)^{-1}Q^{-1}$$

$$U = Q[e^{i\theta}(S - \alpha I)(S - \bar{\alpha} I)^{-1}]Q^{-1}$$

The middle term here is a diagonal matrix

$$e^{i\theta} \begin{pmatrix} \lambda_0 - \alpha & 0 & \dots & 0 \\ 0 & \lambda_1 - \alpha & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \lambda_{n-1} - \alpha \end{pmatrix} \begin{pmatrix} (\lambda_0 - \bar{\alpha})^{-1} & 0 & \dots & 0 \\ 0 & (\lambda_1 - \bar{\alpha})^{-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & (\lambda_{n-1} - \bar{\alpha})^{-1} \end{pmatrix}$$

Thus U is similar to a diagonal matrix of eigenvalues, and the eigenvectors of U are the same as those of P' .

$$U = Q \begin{pmatrix} e^{i\theta} \frac{\lambda_0 - \alpha}{\lambda_0 - \bar{\alpha}} & 0 & \dots & 0 \\ 0 & e^{i\theta} \frac{\lambda_1 - \alpha}{\lambda_1 - \bar{\alpha}} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & e^{i\theta} \frac{\lambda_{n-1} - \alpha}{\lambda_{n-1} - \bar{\alpha}} \end{pmatrix} Q^{-1}$$

Since we had $e^{i\theta}(1 - \alpha)(1 - \bar{\alpha})^{-1} = 1$, 1 is an eigenvalue of U as well as P' and P . Furthermore, U is diagonalized by the same eigenvector matrix Q , so $\sqrt{\pi}$ is the eigenvector corresponding to eigenvalue 1 for U .

Using our formulation of the eigenvalues of P from (4.1), we find the set of eigenvalues of our particular U

$$\lambda_j = e^{i\theta} \frac{\frac{1}{2}\omega_j + \frac{1}{2}\omega_j^{n-1} - \alpha}{\frac{1}{2}\omega_j + \frac{1}{2}\omega_j^{n-1} - \bar{\alpha}}, \quad j = 0 \dots n-1.$$

The corresponding eigenvectors are the columns of Q , which we recall are columns of F_n , the $n \times n$ DFT, if P' is circulant. If P is circulant (but not symmetric), then $Q = DF$, and we can find an explicit formulation for each U_{ij} in terms of the eigenvalues of U and the ratios $\frac{\pi(i)}{\pi(j)}$.

4.3 Extraction of Stationary Vector

Of primary importance is our ability, given a matrix U constructed from stochastic matrix P , to determine the eigenvector $\sqrt{\pi}$. We intend to construct a suitable vector to perform a Fourier transform for the extraction of $\sqrt{\pi}$.

4.3.1 Method

Let $|\psi_0\rangle = \xi_0\sqrt{\pi} + \sum_{k=2}^n \xi_k v_k$, where $\{\sqrt{\pi}, v_2, \dots, v_n\}$ are eigenvectors of U , unknown. Notice that the coefficients ξ_i are inner products of $|\psi_0\rangle$ with the corresponding eigenvector. In particular, notice that ξ_0 is a measure of similarity between the starting vector and $\sqrt{\pi}$. Let $|\psi_t\rangle = U^t|\psi_0\rangle$.

We first concatenate vectors $|\psi_0\rangle||\psi_1\rangle||\dots||\psi_{T-1}\rangle$ to obtain

$$\Psi = \frac{1}{\sqrt{T}} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{T-1} \end{pmatrix}$$

We then multiply by $F_T \otimes I_n$ by $|\psi_0\rangle||\psi_1\rangle||\dots||\psi_{T-1}\rangle$ to obtain

$$F_T \otimes I_n(\Psi) = \frac{1}{\sqrt{T}} \begin{pmatrix} I & I & I & \dots & I \\ I & \omega I & \omega^2 I & \dots & \omega^{T-1} I \\ I & \omega^2 I & \omega^4 I & \dots & \omega^{2(T-1)} I \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ I & \omega^{T-1} I & \omega^{2(T-1)} I & \dots & \omega^{(T-1)^2} I \end{pmatrix} \frac{1}{\sqrt{T}} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{T-1} \end{pmatrix} = \begin{pmatrix} \frac{1}{T} \sum_{t=0}^{T-1} \psi_t \\ \frac{1}{T} \sum_{t=0}^{T-1} \psi_t \omega^t \\ \vdots \\ \vdots \end{pmatrix}$$

We take the first component shown, $\frac{1}{T}(\psi_0 + \psi_1 + \dots + \psi_{T-1})$, which will approach $\xi_0\sqrt{\pi}$ as T approaches infinity as shown in the next section.

It is relevant for practical use to note that this means that sampling from $F_T \otimes I_n(\Psi)$ yields a value in the first n qubits, a value of $\sqrt{\pi}$, with probability $|\xi_0|^2$, the sum of all the squared entries in $\xi_0\sqrt{\pi}$. Thus the magnitude of ξ_0 is related to the efficiency of sampling from $\sqrt{\pi}$. We examine a method for optimizing this process in Section 4.4 with use of statistical priors.

4.3.2 Speed

It is relevant to consider the speed at which the first n qubits, represented in the formula above by $\frac{1}{T} \sum_{t=0}^{T-1} \psi_t(i)$, approaches $\xi_0\sqrt{\pi(i)}$, to determine the accuracy of our approximation relative to the size of T , and we will show that it converges quite quickly. If we look at the evolution of $|\psi_t(i)\rangle$, for eigenvalues $\lambda_0 = 1, \lambda_1 = e^{i\theta_1}, \dots, \lambda_{n-1} = e^{i\theta_{n-1}}$ and initial vector $|\psi_0\rangle$ with unknown eigenvector coefficients $\xi_0, \xi_1, \dots, \xi_{n-1}$,

$$\begin{aligned} |\psi_t(i)\rangle &= \xi_0(1)^t\sqrt{\pi(i)} + \sum_{k=1}^{n-1} \xi_k(\lambda_k)^t v_k(i) \\ &= \xi_0\sqrt{\pi(i)} + \sum_{k=1}^{n-1} \xi_k(e^{i\theta_k})^t v_k(i) \end{aligned}$$

We see that in the average over time, as each eigenvalue not equal to $\lambda_0 = 1$ is a root of unity, for T near a multiple of $2\pi/\theta_k$ the sum of $(1 + e^{i\theta_k} + e^{2i\theta_k} + \dots + e^{(T-1)i\theta_k})$ is near zero.

$$\frac{1}{T} \sum_{t=0}^{T-1} |\psi_t(i)\rangle = \xi_0\sqrt{\pi(i)} + \frac{1}{T} \sum_{k=1}^{n-1} (1 + e^{i\theta_k} + e^{2i\theta_k} + \dots + e^{(T-1)i\theta_k}) \xi_k v_k(i)$$

Furthermore, the absolute value of the eigenvalue sum $\sum \lambda_k^t$, a partial sum of a geometric series, is bounded as follows:

$$\left| \frac{1 - e^{Ti\theta_k}}{1 - e^{i\theta_k}} \right| < \frac{2}{|1 - e^{i\theta_k}|} \quad \text{for } \theta_k \neq 0$$

Thus the quantity $|\sum_{t=0}^{T-1} \lambda_k^t \xi_k v_k(i)|$ is bounded as well, since v_k is a unit vector and $|\xi_k| < 1$:

$$|\xi_k v_k(i) \sum_{t=0}^{T-1} \lambda_k^t| < \frac{2}{|1 - e^{i\theta_k}|} |\xi_k v_k(i)| < \frac{2}{|1 - e^{i\theta_k}|} (1)$$

Therefore the average ($\frac{1}{T}$ multiplied by the sum above) approaches zero on the order of T .

4.4 Accuracy of Algorithm

4.4.1 Statistical Priors

Suppose we would like to have ξ_0 some sufficient size so that we need not run the algorithm in excess to create the $\sqrt{\pi}$ distribution, and we have access, via use of statistical priors, to some stochastic vector $\hat{\pi}$, such that the L_1 error is bounded by some δ , i.e. $\sum_{i=1}^n |\pi(i) - \hat{\pi}(i)| < \delta$.

Lemma 1. *If $\|\pi - \hat{\pi}\|_{L_1} < \delta$, then $\xi_0 > 1 - \delta/2$.*

Proof. Since π and $\hat{\pi}$ are both real vectors, and ξ_0 is uniquely the complex inner product of $\sqrt{\hat{\pi}}$ and $\sqrt{\pi}$,

$$\begin{aligned}
 \xi_0 &= \sum_{i=1}^n \sqrt{\pi(i)} \sqrt{\hat{\pi}(i)} \\
 &= \frac{-1}{2} \sum_{i=1}^n (\sqrt{\pi(i)} - \sqrt{\hat{\pi}(i)})^2 - \pi(i) - \hat{\pi}(i) \\
 &= 1 - \frac{1}{2} \sum_{i=1}^n (\sqrt{\pi(i)} - \sqrt{\hat{\pi}(i)})^2 \\
 &> 1 - \frac{1}{2} \sum_{i=1}^n |\sqrt{\pi(i)} - \sqrt{\hat{\pi}(i)}| (\sqrt{\pi(i)} + \sqrt{\hat{\pi}(i)}) \\
 &= 1 - \frac{1}{2} \|\pi - \hat{\pi}\|_{L_1} \\
 &> 1 - \frac{\delta}{2}
 \end{aligned} \tag{4.3}$$

□

5 Inversion of $(P' - \bar{\alpha}I)$

The efficiency of this algorithm depends fundamentally on the speed with which we can invert the quantity $P - \bar{\alpha}I$. In this paper, we chose to find a closed form for $(P' - \bar{\alpha}I)^{-1}$ and thus U in our specific generated case for the uniform distribution whose matrix is generated in Equation (3.1).

Given that α is a complex number, and the spectrum of P' is real, since it is a positive matrix, $P' - \bar{\alpha}I$ is invertible if P is. To see this, note that P and P' are similar

to each other and the diagonal matrix S of eigenvalues, and letting $Q = (P' - \bar{\alpha}I)^{-1}$ and D be the matrix with entries of π on the diagonal,

$$\begin{aligned} (D^{1/2}PD^{-1/2} - \bar{\alpha}I)Q &= I \\ (D^{1/2}PD^{-1/2} - \bar{\alpha}D^{1/2}D^{-1/2})Q &= I \\ D^{1/2}(P - \bar{\alpha}I)D^{-1/2}Q &= I \\ (P - \bar{\alpha}I)D^{-1/2}QD^{1/2} &= I \end{aligned}$$

Since $\bar{\alpha} \notin \sigma(P)$, $S - \bar{\alpha}I$ is invertible if P is, and similar to $P' - \bar{\alpha}I$, we have shown invertibility of $(P' - \bar{\alpha}I)$.

A couple preliminary notes: as P is a Markov chain, P^T converges to the matrix

$$P^T \rightarrow \begin{pmatrix} \pi(1) & \pi(1) & \dots & \pi(1) \\ \pi(2) & \pi(2) & \dots & \pi(2) \\ \vdots & \vdots & \ddots & \vdots \\ \pi(n) & \pi(n) & \dots & \pi(n) \end{pmatrix}$$

We investigate two potential avenues for insights about the quantity $(P - \alpha I)$: the normalized weighted Laplacian of spectral graph theory, and the complex resolvent $R\{\alpha, P\}$.

From this, we determine that P' has the following behavior:

$$\begin{aligned} P'_{ij} &\rightarrow \frac{\sqrt{\pi(i)}}{\sqrt{\pi(j)}}\pi(i) \\ P'^T &\rightarrow DP_{\sqrt{\pi}}D^{-1} \end{aligned}$$

For matrix (4.1), we can use the calculated eigenvalues and eigenvectors to find the inverse.

$$(P')^{-1} = (F(S - \bar{\alpha})F^{-1})^{-1} = F(S - \bar{\alpha})^{-1}F^{-1}$$

This leads us to the explicit formula for $(P' - \bar{\alpha}I)^{-1}$

$$\begin{aligned} P_{ij}^{-1} &= \frac{1}{n} \sum_{k=0}^{n-1} \omega^{k(i-j)} \lambda_k^{-1} \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \frac{\omega^{k(i-j)}}{\frac{1}{2}\omega^k + \bar{\alpha} + \frac{1}{2}\omega^{k(n-1)}} \\ &= \frac{1}{n} \sum_{k=0}^{n-1} \frac{2\omega^{k(i-j)}}{\omega^k + 2\bar{\alpha} + \omega^{k(n-1)}} \end{aligned}$$

5.1 Fourier Transform

We know that $(P' - \bar{\alpha}I)$ is a circulant matrix, and thus its inverse is circulant. Therefore, we need only determine the first column of the inverse and we will have also determined the remaining entries. Our calculations follow:

$$(P' - \bar{\alpha}I)^{-1}e_0 = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} \iff (P' - \bar{\alpha}I) \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = e_0$$

which implies that

$$1/2a_{n-1} - \bar{\alpha}a_0 + 1/2a_1 = 1 \quad (5.1)$$

$$1/2a_{k-1} - \bar{\alpha}a_j + 1/2a_{j+1} = 0, \forall j \in \{1, 2, \dots, n-1\} \quad (5.2)$$

Applying a QFT to this system of equations, we receive vector

$$\begin{pmatrix} \hat{a}(0) \\ \hat{a}(1) \\ \vdots \\ \hat{a}(n-1) \end{pmatrix}, \hat{a}(k) = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} a_j \omega^{jk}, \omega = e^{2\pi i/n} \quad (5.3)$$

If we multiply equations (4.1) and (4.2) by $\frac{1}{\sqrt{n}}\omega^{jk}$, where j is the index of the a -term multiplied by $\bar{\alpha}$ we have

$$\frac{1}{\sqrt{n}} \left(\frac{a_{n-1}}{2} - \bar{\alpha}a_0 + \frac{a_1}{2} \right) = \frac{1}{\sqrt{n}} \quad (5.4)$$

$$\frac{1}{\sqrt{n}} \left(\frac{\omega^{jk}a_{j-1}}{2} - \omega^{jk}\bar{\alpha}a_j + \frac{\omega^{jk}a_{j+1}}{2} \right) = 0, \forall j \in \{1, 2, \dots, n-1\} \quad (5.5)$$

$$\therefore \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \frac{\omega^{jk}a_{j-1}}{2} - \omega^{jk}\bar{\alpha}a_j + \frac{\omega^{jk}a_{j+1}}{2} = \frac{1}{\sqrt{n}}$$

$$\frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \frac{\omega^{jk}a_{j-1}}{2} = \frac{\omega^k}{2\sqrt{n}} \sum_{j=0}^{n-1} \omega^{(j-1)k} a_{j-1} = \frac{\omega^k \hat{a}(k)}{2}$$

$$\frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \frac{\omega^{jk}a_{j+1}}{2} = \frac{\omega^{-k}}{2\sqrt{n}} \sum_{j=0}^{n-1} \omega^{(j+1)k} a_{j+1} = \frac{\omega^{-k} \hat{a}(k)}{2}$$

$$\therefore \frac{\omega^k \hat{a}(k)}{2} - \bar{\alpha} \hat{a}(k) + \frac{\omega^{-k} \hat{a}(k)}{2} = \frac{1}{\sqrt{n}} \implies \hat{a}(k) = \frac{1}{\sqrt{n} \left(\frac{\omega^k}{2} - \bar{\alpha} + \frac{\omega^{-k}}{2} \right)} \quad (5.6)$$

To get a closed form solution for a_k , we apply the inverse QFT to our vector.

$$\frac{1}{\sqrt{n}} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega^{-1} & \omega^{-2} & \dots & \omega^{-(n-1)} \\ 1 & \omega^{-2} & \omega^{-4} & \dots & \omega^{-2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{-(n-1)} & \omega^{-2(n-1)} & \dots & \omega^{-(n-1)^2} \end{pmatrix} \begin{pmatrix} \hat{a}(0) \\ \hat{a}(1) \\ \hat{a}(2) \\ \vdots \\ \hat{a}(n-1) \end{pmatrix} = \frac{1}{n} \begin{pmatrix} \sum_{j=0}^{n-1} \frac{1}{\frac{\omega^j}{2} - \bar{\alpha} + \frac{\omega^{-j}}{2}} \\ \sum_{j=0}^{n-1} \frac{1}{\frac{\omega^{2j}}{2} - \omega^j \bar{\alpha} + \frac{1}{2}} \\ \sum_{j=0}^{n-1} \frac{1}{\frac{\omega^{3j}}{2} - \omega^{2j} \bar{\alpha} + \frac{\omega^j}{2}} \\ \vdots \\ \sum_{j=0}^{n-1} \frac{1}{\frac{\omega^{nj}}{2} - \omega^{(n-1)j} \bar{\alpha} + \frac{\omega^{(n-2)j}}{2}} \end{pmatrix}$$

$$\implies a_k = \frac{1}{n} \sum_{j=0}^{n-1} \frac{1}{\frac{\omega^{(k+1)j}}{2} - \omega^{kj} \bar{\alpha} + \frac{\omega^{(k-1)j}}{2}} = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \hat{a}(j) \omega^{-kj} \quad (5.7)$$

From here, we will try to find a closed form for a_k and thus find a closed form expression for U in this specific walk, knowing the values of $(P' - \alpha I)$ and $(P' - \bar{\alpha} I)^{-1}$.

5.2 Finding a Closed Form for a_k

We can alternatively characterize the sum $a_k = \frac{1}{n} \sum_{j=0}^{n-1} \dots$ as the following complex integral, where each term in the sum is a residue of a root of unity.

$$\begin{aligned} a_k &= \frac{1}{n} \sum_{j=0}^{n-1} \left(\frac{1}{2} (\omega^{j(k+1)} + \omega^{j(k-1)}) - \omega^{jk} \bar{\alpha} \right)^{-1} \\ &= \frac{1}{n} \sum_{j=0}^{n-1} \frac{1}{2\pi i} \oint_{\partial D(\omega^j, \epsilon)} \left(\frac{1}{2} (z^{(k+1)} + z^{(k-1)}) - z^k \bar{\alpha} \right)^{-1} (z - \omega^j)^{-1} dz \end{aligned}$$

Here by $\oint_{\partial D(\omega^j, \epsilon)}$ we mean the curve integral along the boundary of a disc of radius $\epsilon > 0$ centered at $\omega^j = e^{\frac{2\pi j}{n}}$. We transform the sum of integrals into one large curve integral around the boundary of a large disc centered at 0 with radius R , correcting for the added poles at the roots of the expression $1/2(z + z^{-1}) - \bar{\alpha}$,

$$\gamma_1 = \bar{\alpha} + \sqrt{\bar{\alpha}^2 - 1}, \quad \gamma_2 = \bar{\alpha} - \sqrt{\bar{\alpha}^2 - 1}.$$

For $R \gg 1$, and $\bar{\alpha}$ such that $1 < |\bar{\alpha} + \sqrt{\bar{\alpha}^2 - 1}| < R$, or equivalently $1 < |\bar{\alpha}| < 1/2(R + R^{-1})$,

$$= \frac{1}{2n\pi i} \oint_{|z|=R} \frac{z^k}{1/2(z + z^{-1}) - \bar{\alpha}} \left(\sum_{j=0}^{n-1} \frac{1}{z - \omega^{-j}} \right) dz$$

$$\begin{aligned}
& -\frac{1}{2n\pi i} \oint_{\partial D(\gamma_1, \epsilon)} \frac{z^k}{1/2(z+z^{-1})-\bar{\alpha}} \left(\sum_{j=0}^{n-1} \frac{1}{z-\omega^{-j}} \right) dz \\
& -\frac{1}{2n\pi i} \oint_{\partial D(\gamma_2, \epsilon)} \frac{z^k}{1/2(z+z^{-1})-\bar{\alpha}} \left(\sum_{j=0}^{n-1} \frac{1}{z-\omega^{-j}} \right) dz
\end{aligned}$$

For any n , we have the following identity. Appendix A gives three separate proofs of this fact.

$$\sum_{j=0}^{n-1} \frac{1}{z-\omega^{-j}} = \frac{nz^{n-1}}{z^n-1}.$$

Now let f be the function being integrated, so

$$f = \frac{z^k}{1/2(z+z^{-1})-\bar{\alpha}} \left(\sum_{j=0}^{n-1} \frac{1}{z-\omega^{-j}} \right) = \frac{z^k}{1/2(z+z^{-1})-\bar{\alpha}} \left(\frac{nz^{n-1}}{z^n-1} \right)$$

Substituting $w = \frac{1}{z}$, $dz = -z^2 dw = -w^{-2} dw$, we obtain

$$\begin{aligned}
\oint f(w)dw &= \oint \frac{w^{-k}}{1/2(w+w^{-1})-\bar{\alpha}} \cdot \frac{nw^{1-n}}{w^n-1} - w^{-2} dw \\
&= -2n \oint \frac{1}{(w-\gamma_1)(w-\gamma_2)} \cdot \frac{1}{w^k(1-w^n)} dw \\
a_k &= \frac{1}{2n\pi i} \oint_{|w|=1/R} f(w)dw - \frac{1}{2n\pi i} \oint_{\partial D(\gamma_2, 1/\epsilon)} f(w)dw - \frac{1}{2n\pi i} \oint_{\partial D(\gamma_1, 1/\epsilon)} f(w)dw \\
&= \frac{1}{\pi i} \oint_{|w|=1/R} \frac{1}{(w-\gamma_1)(w-\gamma_2)} \cdot \frac{1}{w^k(1-w^n)} dw \\
&\quad + \frac{1}{\pi i} \oint_{\partial D(\gamma_2, \delta)} \frac{1}{(w-\gamma_1)(w-\gamma_2)} \cdot \frac{1}{w^k(1-w^n)} dw \\
&\quad + \frac{1}{\pi i} \oint_{\partial D(\gamma_1, \delta)} \frac{1}{(w-\gamma_1)(w-\gamma_2)} \cdot \frac{1}{w^k(1-w^n)} dw
\end{aligned} \tag{5.8}$$

We find the following partial fraction decomposition, allowing us to split the first integral into a sum.

$$\begin{aligned}
\frac{1}{(w-\gamma_1)(w-\gamma_2)} &= \frac{1}{2\sqrt{\bar{\alpha}^2-1}} \left(\frac{1}{w-\gamma_1} - \frac{1}{w-\gamma_2} \right) \\
\frac{1}{\frac{1}{2}2\pi i(2\sqrt{\bar{\alpha}^2-1})} &\left[-\oint_{|w|=1/R} \frac{1}{w-\gamma_2} \cdot \frac{1}{w^k(1-w^n)} dw + \oint_{|w|=1/R} \frac{1}{w-\gamma_1} \cdot \frac{1}{w^k(1-w^n)} dw \right]
\end{aligned}$$

To evaluate, we calculate the residue at 0 for each integral. Note that since $R > 1$, the (unit length) roots of $1 - \omega^n$ are not inside the curve $|w| = 1/R$, and $|\gamma_1|, |\gamma_2| > R$:

$$\begin{aligned} & \frac{1}{(k-1)!} \cdot \frac{d^{k-1}}{dw^{k-1}} \left(\frac{1}{(w-\gamma_1)(1-w^n)} \right) \quad \text{evaluated at } w=0 \\ &= \frac{1}{(k-1)!} \frac{d^{k-1}}{dw^{k-1}} \left(\frac{-\gamma_1^{-1}}{1-\frac{w}{\gamma_1}} \cdot \frac{1}{1-w^n} \right) \\ &= \frac{-\gamma_1^{-1}}{(k-1)!} \frac{d^{k-1}}{dw^{k-1}} (1 + \left(\frac{w}{\gamma_1}\right) + \left(\frac{w}{\gamma_1}\right)^2 + \left(\frac{w}{\gamma_1}\right)^3 + \dots)(1 + w^n + w^{2n} + w^{3n} + \dots) \end{aligned}$$

Since $(k-1) < n$, the only term with exponent $k-1$ is $\left(\frac{w}{\gamma_1}\right)^{k-1} \cdot 1$. The $k-1$ th derivative leaves us with $\text{Res}(f, 0) = -\gamma_1^{-k}$.

Similarly, for the other integral, the residue at 0 is $-\gamma_2^{-k}$, so the entire expression is

$$\frac{1}{2\pi i(\sqrt{\bar{\alpha}^2 - 1})} 2\pi i [\gamma_2^{-k} - \gamma_1^{-k}] = \frac{\gamma_1^{-k} - \gamma_2^{-k}}{\sqrt{\bar{\alpha}^2 - 1}}$$

For the curve around γ_2 , there is a simple pole at γ_2 , so

$$\begin{aligned} & \frac{2}{2\pi i} \oint_{\partial D(\gamma_2, 1/\epsilon)} \frac{dw}{(w-\gamma_1)(w-\gamma_2)(w^k)(1-w^n)} = 2\text{Res}(f, \gamma_2) \\ &= 2 \lim_{w \rightarrow \gamma_2} \frac{1}{(w-\gamma_1)(w^k)(1-w^n)} = \frac{-1}{\sqrt{\bar{\alpha}^2 - 1}(\gamma_2^k)(1-\gamma_2^n)} \end{aligned}$$

And similarly,

$$\frac{2}{2\pi i} \oint_{\partial D(\gamma_1, 1/\epsilon)} \frac{dw}{(w-\gamma_1)(w-\gamma_2)(w^k)(1-w^n)} = \frac{1}{\sqrt{\bar{\alpha}^2 - 1}(\gamma_1^k)(1-\gamma_1^n)}$$

So combining all of these,

$$\begin{aligned} 5.8 &= \frac{\gamma_2^{-k} - \gamma_1^{-k}}{\sqrt{\bar{\alpha}^2 - 1}} + \frac{1}{\sqrt{\bar{\alpha}^2 - 1}(\gamma_1^k)(1-\gamma_1^n)} - \frac{1}{\sqrt{\bar{\alpha}^2 - 1}(\gamma_2^k)(1-\gamma_2^n)} \\ &= \frac{(\gamma_2^{-k} - \gamma_1^{-k})(1-\gamma_1^n)(1-\gamma_2^n) + \gamma_1^{-k}(1-\gamma_2^n) - \gamma_2^{-k}(1-\gamma_1^n)}{\sqrt{\bar{\alpha}^2 - 1}(1-\gamma_1^n)(1-\gamma_2^n)} \\ &= \frac{\gamma_1^{n-k} - \gamma_2^{n-k} + \gamma_2^{n-k}\gamma_1^n - \gamma_2^n\gamma_1^{n-k}}{\sqrt{\bar{\alpha}^2 - 1}(1-\gamma_1^n)(1-\gamma_2^n)} \\ a_k &= \frac{\gamma_1^{n-k}}{\sqrt{\bar{\alpha}^2 - 1}(1-\gamma_1^n)} - \frac{\gamma_2^{n-k}}{\sqrt{\bar{\alpha}^2 - 1}(1-\gamma_2^n)} \end{aligned} \tag{5.9}$$

5.3 Finding a Closed Form for U

With this we define $a_m = a_{m \bmod n}$, and then we can describe the inverse of $P' - \bar{\alpha}I$, where the entry $(P - \bar{\alpha}I)_{ij}^{-1} = a_{i-j}$:

$$\begin{pmatrix} a_0 & a_{n-1} & \cdots & a_1 \\ a_1 & a_0 & a_{n-1} & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ a_{n-1} & \cdots & a_1 & a_0 \end{pmatrix}$$

This allows us to find a closed form for U in this case:

$$\begin{aligned} U &= e^{i\theta}(P' - \alpha I)(P' - \bar{\alpha}I)^{-1} \\ &= e^{i\theta} \begin{pmatrix} -\alpha & 1/2 & 0 & \cdots & 1/2 \\ 1/2 & -\alpha & 1/2 & \cdots & 0 \\ 0 & 1/2 & -\alpha & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1/2 & 0 & \cdots & 1/2 & -\alpha \end{pmatrix} \begin{pmatrix} a_0 & a_{n-1} & a_{n-2} & \cdots & a_1 \\ a_1 & a_0 & a_{n-1} & \cdots & a_2 \\ a_2 & a_1 & a_0 & \cdots & a_3 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ a_{n-1} & a_{n-2} & \cdots & a_1 & a_0 \end{pmatrix} \end{aligned}$$

Let $d = (i - j) \bmod n$. Then we use the corresponding modular values a_{d-1}, a_{d+1}, a_d in the following formula.

$$U_{ij} = e^{i\theta}(1/2(a_{d-1} + a_{d+1}) - \alpha \cdot a_d)$$

If $d \neq 0, (n - 1) \bmod n$, then this is equivalent to

$$\begin{aligned} &= \frac{e^{i\theta}}{\sqrt{\bar{\alpha}^2 - 1}} \left(\frac{1}{2} \cdot \left[\frac{\gamma_1^{n-d+1}}{1 - \gamma_1^n} - \frac{\gamma_2^{n-d+1}}{1 - \gamma_2^n} \right] - \alpha \left[\frac{\gamma_1^{n-d}}{1 - \gamma_1^n} - \frac{\gamma_2^{n-d}}{1 - \gamma_2^n} \right] + \frac{1}{2} \cdot \left[\frac{\gamma_1^{n-d-1}}{1 - \gamma_1^n} - \frac{\gamma_2^{n-d-1}}{1 - \gamma_2^n} \right] \right) \\ &= \frac{e^{i\theta}}{\sqrt{\bar{\alpha}^2 - 1}} \left(\frac{(\gamma_2^{n-d}) \frac{1}{2}(\gamma_2 + \gamma_2^{-1}) - \alpha}{1 - \gamma_2^{-n}} - \frac{(\gamma_1^{n-d}) \frac{1}{2}(\gamma_1 + \gamma_1^{-1}) - \alpha}{1 - \gamma_1^{-n}} \right) \end{aligned}$$

Note that since $\gamma_1 = \gamma_2^{-1}$, $\frac{1}{2}\gamma_1 - \alpha + \frac{1}{2}\gamma_1^{-1} = \frac{1}{2}\gamma_2^{-1} - \alpha + \frac{1}{2}\gamma_2 = \bar{\alpha} - \alpha$.

$$U_{ij} = \frac{e^{i\theta}(\bar{\alpha} - \alpha)}{\sqrt{\bar{\alpha}^2 - 1}} \left(\frac{\gamma_2^{n-d}}{1 - \gamma_2^{-n}} - \frac{\gamma_1^{n-d}}{1 - \gamma_1^{-n}} \right)$$

5.4 Arbitrary Circulant Matrices

We now shift our focus from the described n-cycle to circulant matrices which satisfy the previously prescribed conditions:

$$(P' - \bar{\alpha}I) = \begin{pmatrix} c_0 - \bar{\alpha} & c_{n-1} & \dots & c_1 \\ c_1 & c_0 - \bar{\alpha} & \dots & c_2 \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1} & c_{n-2} & \dots & c_0 - \bar{\alpha} \end{pmatrix}$$

Allowing F_n to be the nxn QFT, and using basic results about circulant matrices, we now have the following:

$$(P' - \bar{\alpha}I)^{-1} = F_n D F_n^{-1}, D = \begin{pmatrix} \frac{1}{\sum_{j=0}^{n-1} c_j - \bar{\alpha}} & 0 & \dots & 0 \\ 0 & \frac{1}{\sum_{j=0}^{n-1} c_j \omega^{-j} - \bar{\alpha}} & \dots & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & \dots & 0 & \frac{1}{\sum_{j=0}^{n-1} c_j \omega^{-j(n-1)} - \bar{\alpha}} \end{pmatrix}$$

Thus, in formulating $(P' - \bar{\alpha}I)^{-1}$, we can calculate U easily:

$$\begin{aligned} U &= (P' - \alpha I) F_n D F_n^{-1} \\ &= F_n \begin{pmatrix} \frac{\sum_{j=0}^{n-1} c_j - \alpha}{\sum_{j=0}^{n-1} c_j - \bar{\alpha}} & 0 & \dots & 0 \\ 0 & \frac{\sum_{j=0}^{n-1} c_j \omega^{-j} - \alpha}{\sum_{j=0}^{n-1} c_j \omega^{-j} - \bar{\alpha}} & \dots & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & \dots & 0 & \frac{\sum_{j=0}^{n-1} c_j \omega^{-j(n-1)} - \alpha}{\sum_{j=0}^{n-1} c_j \omega^{-j(n-1)} - \bar{\alpha}} \end{pmatrix} F_n^{-1} \end{aligned}$$

6 Further Questions

6.1 Locality

Definition 4. Suppose there exists some integer $\gamma \in (0, n)$, typically small, such that for each i , we have access only to stationary ratios of the form

$$\frac{\pi(i \pm \epsilon)}{\pi(i)} \quad \text{for } \epsilon < \gamma.$$

We say the algorithm is local if we can determine U_{ij} from only knowledge of P_{ij} , γ -close neighbors in P , and given ratios.

We can certainly construct the entire matrix P' from limited ratio information: each ratio $\frac{\pi(i)}{\pi(j)}$ can be expressed as a (perhaps very long) product of ratios. More efficiently, it can be calculated recursively:

$$P'_{ii} = P_{ii}$$

$$P'_{ij} = P_{ij} \frac{P'_{i(j-1)} P_{(j-1)j}}{P_{i(j-1)} P_{(j-1)j}}$$

We can also calculate an arbitrary stationary vector in the following manner, given reversibility:

$$\frac{\sqrt{\pi(i)}}{\sqrt{\pi(j)}} = \frac{\sqrt{p_{ji}}}{\sqrt{p_{ij}}}$$

$$P'_{ij} = \sqrt{p_{ij} p_{ji}}$$

If the graph itself is local, that is, p_{ij} is negligible for $|j - i| \bmod n > \epsilon$, then this creates a rough diagonal matrix of width ϵ .

However, we would like to be able to ignore as many entries as possible. We therefore pose the following question: is it possible to estimate a small section of U from a small section of P , and corresponding ratios? Or is knowledge of the entire matrix necessary?

A Appendix Proof in Three Methods

We provide here one proof of the equality $\sum_{j=0}^{n-1} \frac{1}{1-\omega^j} = \frac{nz^{n-1}}{z^n-1}$ for n a power of 2, and two proofs showing the equality for any positive integer n .

A.1 Pairing Technique

Suppose $n = 2^\ell$ for some integer ℓ . Noting that $\omega^j = -\omega^{-j}$, take $\frac{1}{z-\omega^{-j}} + \frac{1}{z-\omega^j} = \frac{2z}{z^2-\omega^{2j}}$ for each j , repeat with $\omega^{2j}, \omega^{-2j}$, etc, yielding a final sum of $\frac{2^\ell z^{n-1}}{z^n-1} = \frac{d}{dz} \ln(z^n - 1)$.

A.2 Reverse Partial Fraction Decomposition

Since $z^n - 1 = \prod_{j=0}^{n-1} (z - \omega^j)$, we can express

$$\sum_{j=0}^{n-1} \frac{1}{z - \omega^j} = \frac{S}{z^n - 1}$$

where $S = \sum_{j=0}^{n-1} \prod_{i \neq j} (z - \omega^i)$. We show S is also equivalent to nz^{n-1} . We evaluate this sum as an expansion of

$$\begin{aligned} \sum_{j=0}^{n-1} \prod_{i \neq j} (z - \omega^i) &= \sum_{j=0}^{n-1} \left(z^{n-1} + z^{n-2} \sum_{a \neq j} \omega^a + z^{n-3} \sum_{a \neq b \neq j} \omega^a \omega^b + \dots \right) \\ &= nz^{n-1} + (n-1)z^{n-2} \sum_j \omega^j + (n-2)z^{n-2} \sum_{j \neq i} \omega^i \omega^j + \dots \end{aligned}$$

and show that each sum of the form

$$\sum_{a_1 \neq \dots \neq a_{i-1}} \omega^{a_1} \dots \omega^{a_{i-1}}$$

is equal to 0, thus demonstrating that each term except the leading cancels out.

Lemma 2. Let $\omega = e^{2\pi i/n}$.

a. The sum of unique products of m distinct n^{th} roots of unity not utilizing ω^a is equal to $-\omega^{ma}$

$$\sum_{a \neq j_1 \neq \dots \neq j_m} \omega^{j_1} \dots \omega^{j_m} = (0 - \omega^a)^m$$

b. The sum over all unique products of m distinct n^{th} roots of unity is 0, i.e. for any integer m ,

$$\sum_{\substack{j_1 \neq j_2 \neq \dots \neq j_m \\ j_i \in \{0, 1, \dots, n-1\}}} \omega^{j_1} \omega^{j_2} \dots \omega^{j_m} = 0$$

Proof. a. By Induction. When $m = 1$,

$$\sum_{\substack{j_i \in \{0, 1, \dots, n-1\} \\ j_i \neq a}} \omega^j = \sum_{j=0}^{n-1} \omega^j - \omega^a = 0 - \omega^a$$

Suppose that for some m , Lemma 2.b holds. Then

$$\sum_{a \neq j_1 \neq \dots \neq j_{m+1}} \omega^{j_1} \dots \omega^{j_{m+1}} = \sum_{j_{m+1}=0}^{n-1} \omega^{j_{m+1}} \left(\sum_{j_{m+1} \neq j_1 \neq \dots \neq j_m} \omega^{j_1} \dots \omega^{j_m} \right) - \omega^a \left(\sum_{a \neq j_1 \neq \dots \neq j_m} \omega^{j_1} \dots \omega^{j_m} \right)$$

Which by inductive hypothesis is equal to:

$$= \sum_{j_{m+1}=0}^{n-1} \omega^{j_{m+1}} (-\omega^{mj_{m+1}}) - \omega^a (-\omega^{ma})$$

$$\begin{aligned}
&= (-1)^m \sum_{j_{m+1}=0}^{n-1} \omega^{(m+1)j_{m+1}} - \omega^{(m+1)a} = (-1)^m \frac{1 - (\omega^{m+1})^n}{1 - \omega^{m+1}} - \omega^{(m+1)a} \\
&= (-1)^m (0 - \omega^{(m+1)a}) = (-\omega^a)^{m+1}
\end{aligned}$$

b. By Induction. When $m = 1$, $\sum \omega^j = 0$ by classical result. Suppose for some m ,

$$\sum_{\substack{j_1 \neq j_2 \neq \dots \neq j_m \\ j_i \in \{0, 1, \dots, n-1\}}} \omega^{j_1} \omega^{j_2} \dots \omega^{j_m} = 0.$$

We now consider the sum over $m + 1$ inequal terms. We count them in the following manner

$$\sum_{\substack{j_1 \neq \dots \neq j_m \neq j_{m+1} \\ j_i \in \{0, 1, \dots, n-1\}}} \omega^{j_1} \omega^{j_2} \dots \omega^{j_{m+1}} = \sum_{j_{m+1}=0}^{n-1} \omega^{j_{m+1}} \sum_{j_1 \neq \dots \neq j_m \neq j_{m+1}} \omega^{j_1} \dots \omega^{j_m}$$

From part (a.), we can replace this inner sum:

$$\begin{aligned}
&= \sum_{j_{m+1}=0}^{n-1} \omega^{j_{m+1}} (-\omega^{j_{m+1}})^m = (-1)^m \sum_{j_{m+1}=0}^{n-1} \omega^{(m+1)j_{m+1}} \\
&= (-1)^m \frac{1 - \omega^n}{1 - \omega^{m+1}} = (-1)^m \frac{1 - 1}{1 - \omega^{m+1}} = 0
\end{aligned}$$

□

A.3 Integral

For any n ,

$$\begin{aligned}
\sum_{j=0}^{n-1} \frac{1}{z - \omega^{-j}} &= \frac{d}{dz} \int \sum_{j=0}^{n-1} \frac{1}{z - \omega^{-j}} \\
&= \frac{d}{dz} \sum_{j=0}^{n-1} \int \frac{1}{z - \omega^{-j}} \\
&= \frac{d}{dz} (\ln(z - 1) + \ln(z - \omega) \dots \ln(z - \omega^{n-1})) \\
&= \frac{d}{dz} \ln(z^n - 1) = \frac{nz^{n-1}}{z^n - 1}.
\end{aligned}$$

Thus, we have

$$f = \frac{z^k}{1/2(z + z^{-1}) - \bar{\alpha}} \left(\sum_{j=0}^{n-1} \frac{1}{z - \omega^{-j}} \right) = \frac{z^k}{1/2(z + z^{-1}) - \bar{\alpha}} \left(\frac{nz^{n-1}}{z^n - 1} \right)$$

References

- [1] Lomonaco, Samuel J. Jr., A Rosetta Stone for Quantum Mechanics with an Introduction to Quantum Computation, *Proceedings of Symposia in Applied Mathematics*(2000).
- [2] M.A. Nielsen, I.L. Chuang, *Quantum Computation and Quantum Information, Tenth Anniversary Edition*. Cambridge University Press (2010).
- [3] Zlatko Dimcovic, *Discrete-time Quantum Walks via Interchange Framework and Memory in Quantum Evolution*. Oregon State University (2012).
- [4] David A. Levin, Yuval Peres, Elizabeth L. Wilmer, *Markov Chains and Mixing Times*
- [5] Robert M. Gray, *Toeplitz and Circulant Matrices: A review*, Stanford University
- [6] P. Kurasov and S.T. Kuroda, *Krein's Resolvent Formula and Perturbation Theory*. URL is <http://www2.math.su.se/pak/PDFARCHIV/JOT04.pdf>.
- [7] C. Robin Graham, *Lecture notes for Linear Algebra and Matrix Analysis*. <http://www.math.washington.edu/robin/courses/554.A11/notes/resolvent.pdf>.
- [8] Harry Buhrman, Robert Spalek, *Quantum Verification of Matrix Products*. SODA '06 Proceedings of the seventeenth annual ACM-SIAM symposium on Discrete algorithm (2006).
- [9] Grover L.K., *A fast quantum mechanical algorithm for database search*, Proceedings, 28th Annual ACM Symposium on the Theory of Computing, (May 1996) p. 212.
- [10] Szegedy, Mario. *Quantum speed-up of Markov chain based algorithms*. Foundations of Computer Science, 2004. Proceedings. 45th Annual IEEE Symposium. IEEE (2004).
- [11] N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller, *Equation of State Calculations by Fast Computing Machines*. J. Chem. Phys. 21, 1087 (1953), DOI:10.1063/1.1699114
- [12] W. K. Hastings, *Monte Carlo sampling methods using Markov chains and their applications*. Biometrika (1970) 57 (1): 97-109 doi:10.1093/biomet/57.1.97