Quantum Walks and Mixing

Harmony Zhan

University of Waterloo

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Let A be the adjacency matrix of a graph X. The quantum walk on X is determined by the transition operator

$$U(t) = \exp(itA) = \sum_{k \geq 0} \frac{(itA)^k}{k!}.$$

This is a unitary operator:

$$U(t)\,U(t)^* = \exp(itA)\exp(-itA) = I.$$

On K_2

The adjacency matrix of K_2 satisfies

$$A^{2k} = I, \quad A^{2k+1} = A.$$

Hence

$$\begin{aligned} U(t) &= \sum_{k \geq 0} \frac{(it)^k}{k!} A^k \\ &= \sum_{k \geq 0} \frac{(it)^{2k}}{(2k)!} I + \sum_{k \geq 0} \frac{(it)^{2k+1}}{(2k+1)!} A \\ &= \cos(t) I + i \sin(t) A \\ &= \begin{pmatrix} \cos(t) & i \sin(t) \\ i \sin(t) & \cos(t) \end{pmatrix}. \end{aligned}$$

Evolution

Suppose X has n vertices.

- Quantum system: complex inner product space $\mathbb{C}^n$.
- States: unit vectors in $\mathbb{C}^n$.
- Associate each vertex u with the state e_u.
- Evolution: if the state at time 0 is e_u, then the state at time t is

$$U(t)e_u = \sum_w \alpha_w e_w.$$

- Measurement: $U(t)e_u$ collapses to the state e_v with probability

$$|\langle U(t)e_u, e_v\rangle|^2 = |U(t)_{uv}|^2.$$

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At time $t = \pi/4$,

$$U\left(\frac{\pi}{4}\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}.$$

Uniform Mixing

Definition

We say X admits uniform mixing at time t if $U(t)$ is flat, that is, for all vertices u and v,

$$|U(t)_{u,v}| = \frac{1}{\sqrt{n}}.$$

Computer Plot

How do we determine if a graph admits uniform mixing?

1. Compute the mixing matrix

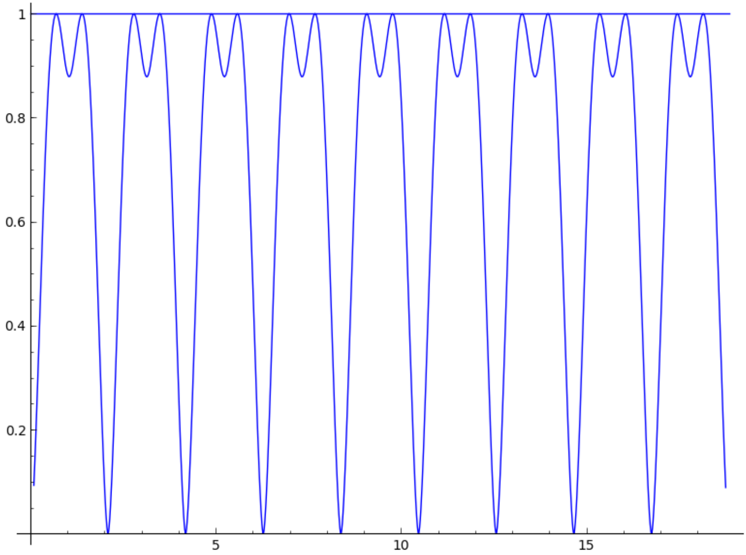
$$M(t) = U(t) \circ U(-t).$$

2. Compute the total entropy of $M(t)$:

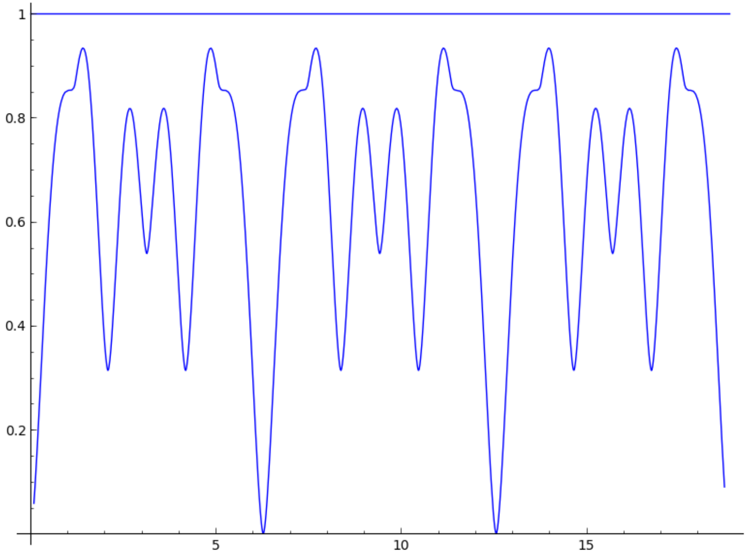
$$-\sum_{i,j} M(t)_{ij} \log(M(t)_{ij})$$

3. Plot the total entropy against t.

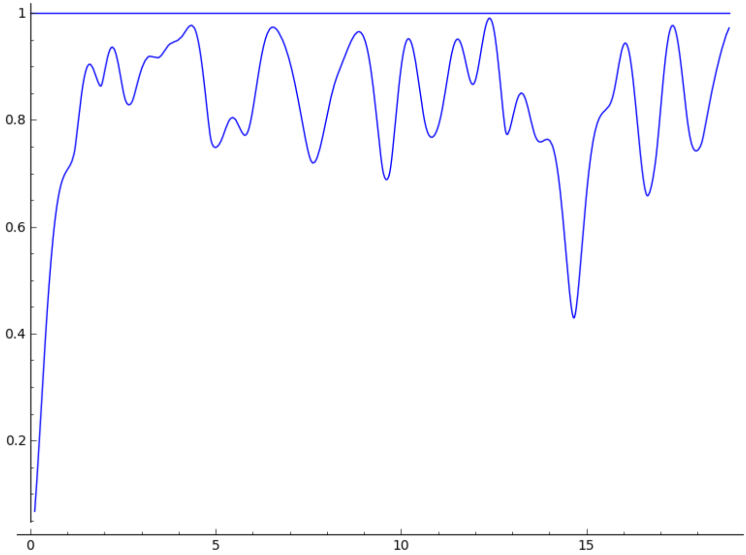
On C_3



On C_6



On C_9



Spectral Decomposition

For every distinct eigenvalue θ_r, let E_r denote the orthogonal projection onto the eigenspace associated with θ_r. Then

$$A = \sum_r \theta_r E_r.$$

If f is a function defined on all the eigenvalues, then

$$f(A) = \sum_r f(\theta_r) E_r.$$

In particular,

$$U(t) = \exp(itA) = \sum_r e^{it\theta_r} E_r.$$

On K_n

The transition matrix of K_n is

$$U(t) = e^{it(n-1)} \frac{1}{n} J + e^{-it} \left(I - \frac{1}{n} J \right).$$

When $n > 4$, for two distinct vertices u and v,

$$|U(t)_{uv}| = \frac{1}{n} |e^{it(n-1)} - e^{-it}| \leq \frac{2}{n} < \frac{1}{\sqrt{n}}.$$

Thus uniform mixing does not occur on the complete graphs with more than 4 vertices.

Known Examples

- K_2 and K_4: at time $\pi/4$; K_3: at time $2\pi/9$ (Ahmadi, Belk, Tamon, Wendler, 2003).

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- Bipartite graphs:

$$U(t) = \begin{pmatrix} K_1(t) & iK_2(t) \\ iK_2(t)^T & K_3(t) \end{pmatrix}$$

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- Strongly regular graphs: completely characterized (Godsil, Mullin and Roy, 2014).

Known Examples

- Cartesian product of X and Y:

$$U_{X \square Y}(t) = U_X(t) \otimes U_Y(t),$$

uniform mixing occurs if and only if both X and Y admits uniform mixing at the same time. The Hamming graphs $H(d, 2), H(d, 3), H(d, 4)$ (Moore and Russell, 2002; Carlson, For, Harris, Rosen, Tamon, and Wrobel, 2007).

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- Cayley graphs over $\mathbb{Z}_q^n$: many examples (Chan, 2013; Mullin, 2013; Zhan, 2014).
- Irregular graphs: $K_{1,3}$ admits uniform mixing at time $2\pi/\sqrt{27}$.

Quotient Graphs of Hamming Graphs

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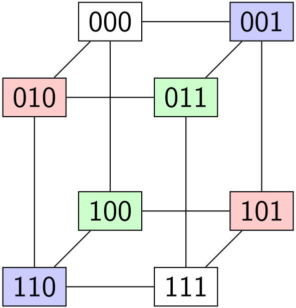
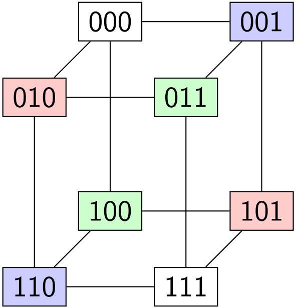


Figure: An equitable partition π.

Every Cayley graph over $\mathbb{Z}_2^d$ or $\mathbb{Z}_3^d$ is a quotient graph of $H(d, 2)$ or $H(d, 3)$.



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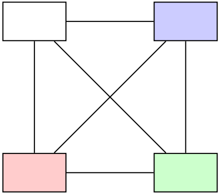

Figure: The quotient graph $H(2, 3)/\langle \mathbf{1} \rangle$ with respect to π.

The entries of the transition matrix of $H(2,3)/\langle \mathbf{1} \rangle$ are block sums of

$U_{H(2,3)}(t) =$

	000	111	001	110	010	101	100	011
000								
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The weight distributions of the cosets of Γ determine whether $H(d,q)/\Gamma$ admits uniform mixing at time $\pi/4$ if $q=2$ or $q=4$, or $2\pi/9$ if $q=3$.

1. We have a complete characterization of $H(d,2)/\langle a\rangle$ and $H(d,2)/\langle a,b\rangle$ which admit uniform mixing at time $\pi/4$, in terms of the generators (Mullin, 2013).
2. We have a complete characterization of $H(d,3)/\langle a\rangle$ and $H(d,3)/\langle a,b\rangle$ which admit uniform mixing at time $2\pi/9$, in terms of the generators (Zhan, 2014).

Faster Mixing in Hamming Schemes

Suppose $A(X)$ is in the Bose-Mesner algebra of $\mathcal{H}(d, q)$. If X admits uniform mixing at time τ, then $U(\tau)$ is a multiple of a complex Hadamard matrix.

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Suppose $A(X)$ is in the Bose-Mesner algebra of $\mathcal{H}(d,q)$. If X admits uniform mixing at time τ, then $U(\tau)$ is a multiple of a complex Hadamard matrix.

1. Guess the complex Hadamard matrix:

$$e^{i\beta}\begin{pmatrix}1 & i\\ i & 1\end{pmatrix}^{\otimes d}.$$

2. Derive conditions on the eigenvalues of X, for the above matrix to be achieved by $U_X(t)$.
3. Find X.

Faster Mixing in Hamming Schemes

1. For $k \geq 2$ and $r \in \{2^{k+1}-7, 2^{k+1}-5, 2^{k+1}-3, 2^{k+1}-1\}$, the r-distance graphs X_r of the Hamming graph $H(2^{k+2}-8, 2)$ admit uniform mixing at time $\pi/2^k$ (Chan, 2013).

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2. For $k \geq 2$ and $r \in \{3^k - 1, 3^k - 4, 3^k - 7\}$, the r-distance graphs X_r of the Hamming graph $H(2 \cdot 3^k - 9, 3)$ admit uniform mixing at time $2\pi/3^k$ (Zhan, 2014).

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3. In the Hamming scheme $\mathcal{H}(2k+1, 3)$, the graph with adjacency matrix

$$\sum_{\ell} A_{3\ell+i}$$

has uniform mixing at time $2\pi/3^k$ (Godsil and Zhan, 2017).

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3. In the Bose-Mesner algebra of $\mathcal{H}(d, q)$, is there a bound of the mixing time in terms of the size of the graph?
4. If X admits uniform mixing at time t, is it true that $t\theta_r$ is a rational multiples of π, for all eigenvalues θ_r of X?