Quantum Walks and Mixing

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August 7, 2017
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:

$$U(t)U(t)^* = \exp(itA)\exp(-itA) = I.$$
The adjacency matrix of $K_2$ satisfies

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

Hence

$$U(t) = \sum_{k \geq 0} \frac{(it)^k}{k!} A^k$$

$$= \sum_{k \geq 0} \frac{(it)^{2k}}{(2k)!} I + \sum_{k \geq 0} \frac{(it)^{2k+1}}{(2k+1)!} A$$

$$= \cos(t) I + i \sin(t) A$$

$$= \begin{pmatrix} \cos(t) & i \sin(t) \\ i \sin(t) & \cos(t) \end{pmatrix}.$$
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
  \[ \left| \langle U(t) e_u, e_v \rangle \right|^2 = \left| U(t)_{uv} \right|^2. \]
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At time $t = \pi/4$,

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

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

$$|U(t)_{u,v}| = \frac{1}{\sqrt{n}}.$$
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 $\theta_r$, let $E_r$ denote the orthogonal projection onto the eigenspace associated with $\theta_r$. 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,

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

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).

- Bipartite graphs: $U(t) = K_1(t) \cup K_2(t) \cup K_3(t)$ if uniform mixing occurs then $n = 2$ or $n$ is divisible by 4 (Mullin, 2013).

- Strongly regular graphs: completely characterized (Godsil, Mullin and Roy, 2014).
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$$U(t) = \begin{pmatrix} K_1(t) & iK_2(t) \\ iK_2(t)^T & K_3(t) \end{pmatrix}$$

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

**Figure:** An equitable partition \( \pi \).

**Figure:** The quotient graph \( H(2, 3)/\langle 1 \rangle \) with respect to \( \pi \).
The entries of the transition matrix of $H(2, 3)/\langle 1 \rangle$ are block sums of

$$
U_{H(2, 3)}(t) = \begin{pmatrix}
000 & 111 & 001 & 110 & 010 & 101 & 100 & 011 \\
000 & 111 & 001 & 110 & 010 & 101 & 100 & 011 \\
001 & 110 & 010 & 101 & 100 & 011 & 000 & 111 \\
011 & 100 & 001 & 110 & 010 & 101 & 100 & 011 \\
101 & 010 & 001 & 110 & 010 & 101 & 100 & 011 \\
110 & 010 & 001 & 110 & 010 & 101 & 100 & 011 \\
100 & 010 & 001 & 110 & 010 & 101 & 100 & 011 \\
011 & 100 & 001 & 110 & 010 & 101 & 100 & 011
\end{pmatrix}
$$
The weight distributions of the cosets of $\Gamma$ 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).
Suppose $A(X)$ is in the Bose-Mesner algebra of $\mathcal{H}(d, q)$. If $X$ admits uniform mixing at time $\tau$, then $U(\tau)$ is a multiple of a complex Hadamard matrix.
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 $\tau$, then $U(\tau)$ is a multiple of a complex Hadamard matrix.

1. Guess the complex Hadamard matrix:

$$e^{i\beta} \left( \begin{array}{cc} 1 & i \\ i & 1 \end{array} \right)^{\otimes d}.$$

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

3. Find $X$. 
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).
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).

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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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).
Open Problems

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4. If $X$ admits uniform mixing at time $t$, is it true that $t\theta_r$ is a rational multiples of $\pi$, for all eigenvalues $\theta_r$ of $X$?