Average mixing of continuous quantum walks

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This is a presentation of:

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Outline

1) Background and Definitions, particularly, the average mixing matrix (AMM)
2) How to work with the AMM
3) The AMM of paths
4) The AMM and cospectral vertices
Let $X$ be a graph on $V(X) = \{1, \ldots, n\}$ vertices with adjacency matrix $A$. We will be considering the operator

$$H(t) = \exp(\imath tA) = \sum_{k=0}^{\infty} \frac{1}{k!} (\imath tA)^k$$

where $t \in \mathbb{R}$. The idea is that $H(t)$ determines a \textbf{continuous quantum walk} by associating the standard basis vector $e_i \in \mathbb{C}^n$ with the vertex $i$. Doing so, yields that

$$|e_u^T H(t) e_v|^2$$

is the probability that the quantum walk starting at vertex $v$ is at vertex $u$ at time $t$. 
The Schur Product of two $n \times m$ matrices $A, B$, denoted by $A \circ B$, is the entry-wise product of $A$ and $B$. Then define the following:

$$M_X(t) := H(t) \circ H(-t)$$

$$\hat{M}_X := \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} M_X(t) dt$$

The matrix $\hat{M}_X$ is the average mixing matrix of $X$. The goal is to relate properties of $\hat{M}_X(t)$ to $X$. 
Properties of the Matrix Exponential

There are a few properties of the matrix exponential that are useful for us. Let $B, C$ be complex square matrices.

1) If $B$ is skew hermitian, then $\exp(B)$ is unitary.
2) If $BC = CB$, then $\exp(B + C) = \exp(B)\exp(C)$.
3) If $B$ is idempotent, then
   \[ \exp B = \sum_{k=0}^{\infty} \frac{1}{k!} B^k = I + \left( \sum_{k=1}^{\infty} \frac{1}{k!} \right) B = I + (e - 1)P \]

Property 1) gives us that $H(t) = \exp(\imath tA)$ is unitary in virtue of

\[ (\imath tA)^* = -\imath tA \]
Recall that the spectral decomposition of $A$ is given by

$$A = \sum_r \theta_r E_r$$

where $E_r$ is idempotent. Then we have:

$$H(t) = \sum_r \exp(\imath t \theta_r) E_r$$

$$M_X(t) = \sum_r E_r \circ E_r + 2 \sum_{r \leq s} \cos((\theta_r - \theta_s)t) E_r \circ E_s$$

**Lemma**

If $A = \sum_r \theta_r E_r$, then

$$\hat{M}_X = \sum_r E_r \circ E_r.$$
Lemma

If $X$ is connected, then all entries of $\hat{M}_X$ are positive.

Proof.

Notice that $E_r \circ E_r$ is nonnegative.
Suppose $(\hat{M}_X)_{u,v} = 0$. This implies $(E_r \circ E_r)_{u,v} = 0$ for all $r$.
Furthermore, this implies that $(E_r)_{u,v} = 0$ for all $r$.
Recall that $A$ is a linear combination of $E_r$ and $E_i E_j = 0$ for $i \neq j$.
Therefore, $(A^k)_{u,v} = 0$ for all $k$, and $X$ is disconnected. □
Lemma

The idempotents of $E_1, \ldots, E_n$ in the spectral decomposition of $P_n$ are given by

$$(E_r)_{j,k} = \frac{2}{n+1} \sin \left( \frac{jr \pi}{n+1} \right) \sin \left( \frac{kr \pi}{n+1} \right).$$

Proof.

Recall that the adjacency eigenvalues of $P_n$ are $2 \cos(\beta)$ with eigenvectors $z(\beta) = \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix}$ where $\beta$ ranges over

$$\beta = \frac{\pi r}{n+1}, \ r \in [n].$$

To be continued…
If $\lambda$ is a simple eigenvalue with vector $x$, then $\frac{1}{x^Tx}xx^T$ is the projection onto the eigenspace of $\lambda$.

proof continued.

Using the fun fact, we get that $\frac{1}{z(\beta)^Tz(\beta)} = \frac{2}{n+1}$ and

$$(z(\beta)z(\beta)^T)_{j,k} = \sin(j\beta)\sin(k\beta) = \sin\left(\frac{jr\pi}{n+1}\right)\sin\left(\frac{kr\pi}{n+1}\right).$$
Lemma

If $E_1, \ldots, E_n$ are idempotents for $P_n$, then

$$\hat{M}_{P_n} = \sum_r E_r \circ E_r = \frac{1}{2n+2}(2J + I + J).$$

Proof.

By the previous Lemma we have

$$(E_r \circ E_r)_{j,k} = \frac{4}{(n+1)^2} \sin^2 \left( \frac{j \pi}{n+1} \right) \sin^2 \left( \frac{k \pi}{n+1} \right).$$

Using some trigonometry we get...
proof continued.

\[(n + 1)^2 (E_r \circ E_r)_{j,k} =
1 - \cos \left(\frac{2jr\pi}{n+1}\right) - \cos \left(\frac{2kr\pi}{n+1}\right) + \frac{1}{2} \cos \left(\frac{2(j+k)r\pi}{n+1}\right) + \frac{1}{2} \cos \left(\frac{2(j-k)r\pi}{n+1}\right)\].

Summing across \(r\) and using the fact that \(\sum_{r=1}^{n} \cos \left(\frac{2lr\pi}{n+1}\right) = -1\), the right hand side (RHS) evaluates to

\[
RHS = \begin{cases} 
3(n + 1)/2 & j = k; \\
3(n + 1)/2 & j + k = n + 1; \\
2n + 2 & j = k, j + k = n + 1; \\
n + 1 & \text{otherwise.}
\end{cases}
\]

\[\square\]
An Example: $P_3$

Recall that the eigenvalues of $P_3$ are $0, \sqrt{2}, -\sqrt{2}$ with corresponding vectors $[1, 0, -1]^T, [1, \sqrt{2}, 1]^T, [1, -\sqrt{2}, 1]^T$. These are all simple eigenvalues, so the corresponding projections are

$$E_1 = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad E_2 = \begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}$$

$$E_3 = \begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}$$

Then

$$\hat{M}_{P_3} = E_1/2 + E_2/4 + E_3/4 = \begin{pmatrix} 3/8 & 2/8 & 3/8 \\ 2/8 & 4/8 & 2/8 \\ 3/8 & 2/8 & 3/8 \end{pmatrix}$$
Theorem

Let $X$ be a graph with vertices $u$ and $v$, and let $E_1, \ldots, E_m$ be the idempotents in the spectral decomposition of $A(X)$. TFAE:

1) $(A^k)_{u,u} = (A^k)_{v,v}$ for all $k \geq 0$
2) $\|E_re_u\|^2 = \|E_re_v\|^2$
3) The graphs $X - u$ and $X - v$.

If any of the conditions above hold for vertices $u$ and $v$, we say that $u$ and $b$ are cospectral. Furthermore, if $E_re_u = \pm E_re_v$ for all $r$, then we say that $u$ and $v$ are strongly cospectral.

Lemma

If $u$ and $V$ are vertices in $X$ and the eigenvalues of $X$ are all simple, then $U$ and $v$ are strongly cospectral if and only if they are cospectral.
Theorem

Let \( \hat{M}_X \) be the average mixing matrix of the graph \( X \). Then vertices \( u \) and \( v \) are strongly cospectral if and only if \( \hat{M}_X(e_v - e_u) = 0 \).

Proof.

Some algebra shows that if \( N \) is PSD and \( N(e_u - e_v) = 0 \), then \( N[v, u](e_u - e_v) = 0 \).

\( \hat{M}_X(e_u - e_v) = 0 \) implies

\[
0 = (e_u - e_v)^T \hat{M}_X(e_u - e_v) = \sum_r (e_u - e_v)^T (E_r \circ E_r)(e_u - e_v).
\]

Notice that each summand \( E_r \circ E_r \) is PSD, so we have

\[
(E_r \circ E_r)(e_u - e_v) = 0 \quad \text{for all} \quad r.
\]

This implies

\[
((E_r)_{u,u})^2 = ((E_r)_{u,v})^2 = ((E_r)_{v,v})^2.
\]

Applying Cauchy-Schwarz gives that

\[
E_re_u = \pm E_re_v.
\]
Returning to our Example

Recall that the average mixing matrix of $P_3$ is

$$\hat{M}_{P_3} = \begin{pmatrix} \frac{3}{8} & \frac{2}{8} & \frac{3}{8} \\ \frac{2}{8} & \frac{4}{8} & \frac{2}{8} \\ \frac{3}{8} & \frac{2}{8} & \frac{3}{8} \end{pmatrix}.$$  

The first and last row are equal, and $P_3$ has all simple eigenvalues. Therefore, $P_3 - v_1$ and $P_3 - v_3$ are cospectral.
Thank you!