Average Mixing Matrices

Chris Godsil, University of Waterloo

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Outline

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1. A Quantum Walk
   - The Transition Matrix

2. Mixing
   - Instantaneous Mixing
   - Average Mixing

An Operator

Definition

Let X be a graph with adjacency matrix A. We define the transition matrix $H_A(t)$ by

$$H_A(t) := \exp(itA)$$

Example

Suppose $X = K_2$. Then $A^2 = I$ and so

$$\begin{aligned} H_A(t) &= I + itA - \frac{1}{2}t^2 I - \frac{1}{6}t^3 A + \frac{1}{24}t^4 I + \cdots \\ &= \cos(t)I + i\sin(t)A \\ &= \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix} \end{aligned}$$

Properties of the Transition Operator

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- $H_A(t)$ is unitary.

Mixing

Definition

We define the mixing matrix $M_A(t)$ by

$$M_A(t) := H(t) \circ H(-t).$$

Example

If $X = K_2$ then

$$M_A(t) = \begin{pmatrix} \cos^2(t) & \sin^2(t) \\ \sin^2(t) & \cos^2(t) \end{pmatrix}.$$

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- It's all that we can actually observe of a continuous quantum walk.

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Instantaneous Uniform Mixing

Definition

We have instantaneous uniform mixing at time t if

$$M(t) = \frac{1}{|V(X)|} J.$$

Example

We have instantaneous uniform mixing on K_2 at time $\pi/4$.

Hadamard Matrices

If we have instantaneous uniform mixing at t, then $H(t)$ is a flat unitary matrix, i.e., all its entries have the same absolute value. Physicists refer to such matrices a generalized Hadamard matrices.

The Cartesian Product

Definition

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$$A(X) \otimes I + I \otimes A(Y).$$

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Corollary

There is instantaneous uniform mixing on the d-cube at time $\pi/4$.

Instantaneous Mixing is Rare?

Theorem (Chan, Roy)

Instantaneous mixing cannot occur on a strongly regular graph.

Outline

The Average Mixing Matrix

Definition

The average mixing matrix $\widehat{M}_X$ of X is given by

$$\widehat{M}_X = \frac{1}{T}\int_0^T M(t)\,dt.$$

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- If X is connected, $\widehat{M}_X > 0$.
- If $X \neq K_2$, the average mixing matrix is not equal to $\frac{1}{n}J$.

Spectral Decomposition

If A has the spectral decomposition

$$A = \sum_r \theta_r E_r$$

then

$$H_A(t) = \sum_r e^{it\theta_r} E_r.$$

Lemma

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

A Formula for the Average Mixing Matrix

Theorem

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Corollary

$$\widehat{M}_X \succcurlyeq 0.$$

Average Mixing on Paths

Let $T = T_n$ be the permutation matrix that swaps i and $n+1-i$ for $i = 1, \dots, n$.

Lemma

If P is the path on n vertices, then its average mixing matrix is

$$\frac{1}{2n+2}(2J + I + T).$$

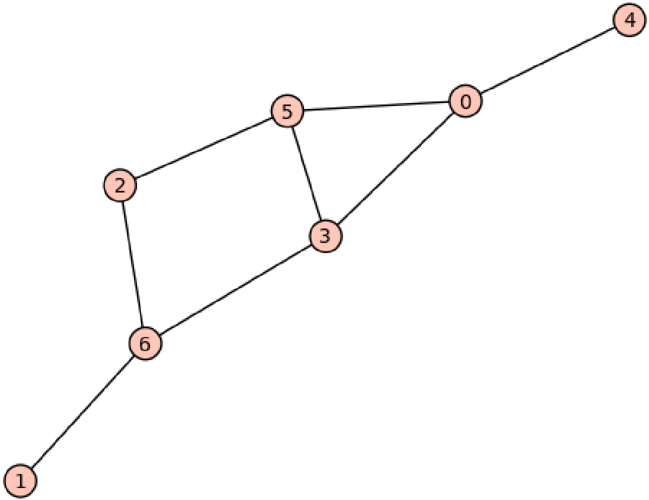
Average Mixing on Cycles

Lemma

If n is odd, the average mixing matrix for C_n is

$$\frac{n-1}{n^2}J + \frac{1}{n}I.$$

The Complement of a Graph. . .



. . . and its Average Mixing Matrix

$$\begin{pmatrix} 0.4442 & 0.0808 & 0.0664 & 0.0854 & 0.1362 & 0.0849 & 0.1019 \\ 0.0808 & 0.2474 & 0.1025 & 0.0964 & 0.1582 & 0.1540 & 0.1607 \\ 0.0664 & 0.1025 & 0.2273 & 0.2233 & 0.1438 & 0.1221 & 0.1146 \\ 0.0854 & 0.0964 & 0.2233 & 0.2346 & 0.1231 & 0.1149 & 0.1222 \\ 0.1362 & 0.1582 & 0.1438 & 0.1231 & 0.2015 & 0.1532 & 0.0840 \\ 0.0849 & 0.1540 & 0.1221 & 0.1149 & 0.1532 & 0.2029 & 0.1680 \\ 0.1019 & 0.1607 & 0.1146 & 0.1222 & 0.0840 & 0.1680 & 0.2487 \end{pmatrix}$$

Rationality

Theorem

The average mixing matrix of a graph is rational.

Discriminants

Lemma

If D is the discriminant of the minimal polynomial of $A(X)$ and $\widehat{M}_X$ is its average mixing matrix, then $D^2\widehat{M}_X$ is an integer matrix. If the eigenvalues of X are simple, $D\widehat{M}_X$ is simple.

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For our 7-vertex example, the eigenvalues are simple and

$$D = 2^6 \times 8438040749$$

and 2×8438040749 times $\widehat{M}_X$ is rational???

The End(s)