Graph Spectra and Quantum State Transfer

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Outline

1. State Transfer
   - Some Physics
   - Periodicity
   - The Ratio Condition
   - Cubelike Graphs
   - Cospectral Vertices
2. Mixing
   - Probability
   - Pretty Good State Transfer
   - Average Mixing

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Cosmology

Quote

Hydrogen is a colorless, odorless gas which given sufficient time, turns into people. (Henry Hiebert)

Axioms

Quote

“The axioms of quantum physics are not as strict as those of mathematics”

The Transition Matrix

Definition

Let X be a graph with adjacency matrix A. The transition matrix associated with X is

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

An Example

We consider $X = K_2$. Then

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and $A^2 = I$ and

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

Some Properties of $H_A(t)$

- $H_A(t)$ is symmetric.
- $\overline{H_A(t)} = H_A(-t)$, so $H(t)$ is unitary.
- $H_A(t) \circ H_A(-t)$ is a doubly stochastic matrix.

Perfect State Transfer

Definition

The graph X admits perfect state transfer from the vertex u to the vertex v at time τ if there is a complex number γ of norm 1 such that

$$H_A(\tau)e_u = \gamma e_v.$$

Perfect State Transfer on P_2...

If $X = K_2$ then

$$H_A(t) = \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix}$$

whence

$$H_A(\pi/2) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

and

$$H_A(\pi/2)e_1 = ie_2.$$

. . . and on P_3

For P_3, we have perfect state transfer between the two end vertices at time

$$\tau = \frac{\pi}{2\sqrt{2}}.$$

Two Products

If $X \square Y$ is the Cartesian product of X and Y, then

$$H_{X \square Y}(t) = H_X(t) \otimes H_Y(t).$$

The Cartesian product of P_m and P_n is an $n \times n$ grid.

Cartesian Powers

Lemma

If we have perfect state transfer at time τ on X and on Y, we have perfect state transfer on $X \square Y$ at time τ.

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Corollary

There is perfect state transfer between each pair of antipodal vertices in the d-cube at time $\pi/2$. And between antipodal vertices in $P_3^{\square d}$ at time $\pi/2\sqrt{2}$.

A Reference

Matthias Christandl, Nilanjana Datta, Tony C. Dorlas, Artur Ekert, Alastair Kay, Andrew J. Landahl:
"Perfect Transfer of Arbitrary States in Quantum Spin Networks"

arXiv:quant-ph/0411020v2

Outline

A Symmetry Condition

If

$$H_A(\tau)e_u = \gamma e_v.$$

then taking complex conjugates yields

$$H_A(-\tau)e_u = \bar{\gamma} e_v$$

and therefore

$$H_A(\tau)e_v = \gamma e_v.$$

Periodicity at a Vertex

Definition

The graph X is periodic at the vertex u if there is a time τ such that $H_A(\tau)e_u = \gamma e_u$ (where $|\gamma| = 1$). We say X itself is periodic if X is periodic at each vertex, with the same period τ.

We have seen that P_2 is periodic.

Perfect State Transfer Implies Periodicity at a Vertex

Lemma

If there is perfect state transfer from u to v in X at time τ, then X is periodic at u and v with period 2τ.

Spectral Decomposition

Suppose A is symmetric. Then it has the spectral decomposition

$$A = \sum_r \theta_r E_r$$

where θ_r runs over the distinct eigenvalues of A and E_r represents orthogonal projection onto the eigenspace $\ker(A - \theta_r I)$.

Recall that $\sum_r E_r = I$ and $E_r E_s = \delta_{r,s} E_r$. The spectral decomposition of $H_A(t)$ is

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

Periodicity and Integer Eigenvalues

Lemma

If the eigenvalues of X are integers, then X is periodic with period dividing 2π.

Proof.

If the eigenvalues of X are integers then $e^{2\pi i\theta_r} = 1$ and

$$H_A(2\pi) = \sum_r e^{2\pi i\theta_r} E_r = \sum_r E_r = I.$$

□

Although the eigenvalues of P_3 are not integers, P_3 is periodic.

Perfect State Transfer on Vertex-Transitive Graphs

Theorem

If X is connected and vertex transitive and we have pst at time τ with phase γ then $|V(X)|$ is even and $\gamma^{-1}H(\tau) \in \mathrm{Aut}(X)$.

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Eigenvalue Support

Suppose $H(\tau)e_u = \gamma e_u$ where $|\gamma| = 1$. Then

$$\gamma E_r e_u = E_r H(\tau) e_u = e^{i\theta_r \tau} E_r e_u$$

and it follows that if $(E_r)_{u,u} \neq 0$ then $e^{i\theta_r \tau} = \gamma$.

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Definition

If $u \in V(X)$, the eigenvalue support $\mathrm{esupp}(u)$ of u is the set

$$\{\theta_r : (E_r)_{u,u} \neq 0\}.$$

A Rational Ratio

Theorem

If X is periodic at u and θ_a, θ_b, θ_r, θ_s are eigenvalues in the eigenvalue support of u and $\theta_a \neq \theta_b$, then

$$\frac{\theta_r - \theta_s}{\theta_a - \theta_b} \in \mathbb{Q}.$$

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Proof.

If $e^{i\theta_r \tau} = e^{i\theta_s \tau}$, there is an integer $m_{r,s}$ such that

$$(\theta_r - \theta_s)\tau = 2\pi m_{r,s}.$$

An analogous equation holds for θ_a and θ_b. □

Integrality, Almost

Theorem (Godsil)

If $\delta = |\operatorname{esupp}(u)|$ *and we have* uv*-pst in* X*, then*

(a) $3 \leq \delta < |V(X)|$

(b) *either all eigenvalues in* $\operatorname{esupp}(u)$ *are integers, or*

(c) X *is bipartite and all eigenvalues in* $\operatorname{esupp}(u)$ *are of the form* $\frac{1}{2}(a_i + b_i\sqrt{\Delta})$*, where* Δ *is a square-free integer and* a_i, b_i *are integers.*

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Corollary

For each integer k there are only finitely many graphs with maximum valency at most k where pst occurs.

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Definition

Let C be a set of non-zero vectors in $\mathbb{Z}_2^d$. Then $X(C)$ is the graph with vertex set $\mathbb{Z}_d$, where two vectors are adjacent if their difference is in C. We say X is a cubelike graph.

Example

If C is the standard basis $e_1, \ldots, e_d$ then $X(C)$ is the d-cube.

Decomposing Adjacency Matrices

If $X(C)$ cubelike and $m = |C|$, then each element of C determines a perfect matching of $X(C)$; denote the adjacency matrices of these matchings by $P_1, \ldots, P_m$. Then $P_i^2 = I$ and $P_i P_j = P_j P_i$ and $\mathrm{tr}(P_i) = 0$ and

$$A = P_1 + \cdots + P_m$$

and therefore

$$H_X(t) = \exp(it(P_1 + \cdots + P_m)) = \prod_r \exp(itP_r)$$

Euler Communicates

We know that

$$\exp(it) = \cos(t) + i\sin(t)$$

and the same proof yields that

$$\exp(itP_r) = \cos(t)I + i\sin(t)P_r.$$

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Theorem (Bernasconi, Godsil, Severini)

A cubelike graph with connection set C admits pst at time $\pi/2$ if and only if the sum of the elements of C is not zero, that is, if and only if $M_C\mathbf{1} \neq 0$.

Outline

Projections

Lemma

If we have perfect state transfer from u to v then for each r,

$$E_r e_u = \pm E_r e_v.$$

Proof.

Write H for $H(\tau)$ and suppose $He_u = \gamma e_v$. Then

$$\gamma E_r e_v = E_r H e_u = e^{i\theta_r \tau} E_r e_u$$

and thus $E_r e_v = \gamma^{-1} e^{i\theta_r \tau} E_r e_u$. Since e_u and e_v are real and $|\gamma^{-1} e^{i\theta_r \tau}| = 1$, we're done. □

Characterizing Cospectral Vertices

Theorem

For two vertices u and v in the graph X, the following statements are equivalent:

- $X \setminus u$ *and* $X \setminus v$ *are cospectral.*
- *For each idempotent* E_r *we have* $\|E_r e_u\| = \|E_r e_v\|$.
- *The generating function for the closed walks in* X *that start at* u *is equal to the generating function for the closed walks in* X *that start at* v.

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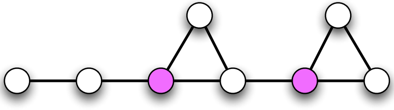
Note that

$$\|E_r e_u\|^2 = e_u^T E_r e_u = (E_r)_{u,u}.$$

If $E_r e_u = \pm E_r e_v$ for all r, we say that u and v are strongly cospectral.

An Example



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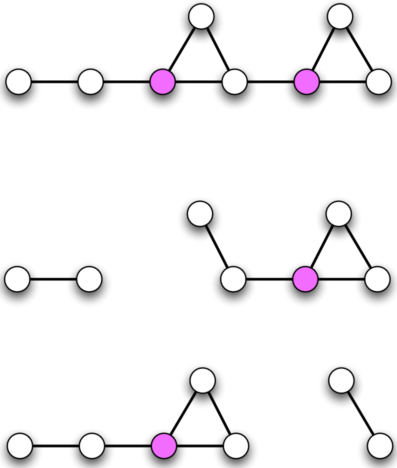

Outline

A Doubly Stochastic Matrix

Definition

If $H(t)$ is a transition matrix, we define $M(t)$ by

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

Thus we get $M(t)$ by replacing each entry of $H(t)$ by the square of its absolute value. Since $H(t)$ is unitary each row and column of $M(t)$ sums to 1, and thus specifies a probability distribution.

New Questions

Asking if we have uv-pst on X at time τ is asking if the probability density given by the u-row of $M(\tau)$ is concentrated on v. We are going to look at some variants of this question.

Outline

State Transfer on Paths

In their fundamental paper on state transfer, Christandl et al proved that perfect state transfer between end vertices does not occur on paths with more than three vertices.

We know now that, if $n \geq 4$, pst does not take place at all on the path P_n (Stevanović, Godsil).

Near Misses

- Computation yields that the first row of $M_{P_4}(305\pi)$ is equal to

$$(0.000000265, 0.0000000000, 0.0000010609, 0.9999986738)$$

and it can be shown that the first row of $M_{P_4}(t)$ gets arbitrarily close to e_4 infinitely often.

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  and it can be shown that the first row of $M_{P_4}(t)$ gets arbitrarily close to e_4 infinitely often.
- It seems possible that we always have "pretty good" state transfer between the end vertices of a path.
- Casaccino et al have "numerical evidence" that we can always get pst between the end vertices of a path by adding loops of the right weight to its end vertices.

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The Average Mixing Matrix

Definition

The average mixing matrix is

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

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Lemma

$$\widehat{M} = \sum_r E_r^{\circ 2}.$$

Average Mixing is not Uniform

Theorem (Godsil)

If X is a graph on n vertices and $\widehat{M} = n^{-1}J$, then $n \le 2$.

Proof.

The matrices $E_r^{\circ 2}$ are positive semidefinite and so if their sum has rank one then $\mathrm{rk}(E_r^{\circ 2}) = 1$ for all r. Hence any two vertices in X are cospectral and all eigenvalues of X are simple. □

Paths

Theorem (Godsil)

Let $T = T_n$ be the permutation matrix such that $Te_i = e_{n+1-i}$ for all i. The average mixing matrix for P_n is

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

Odd Cycles

Theorem

If n is odd then the average mixing matrix for the cycle C_n is

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

Rationality

Theorem (Godsil)

The average mixing matrix of a graph is rational.

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The average mixing matrix of a graph is rational.

If D is the discriminant of the minimal polynomial of A then $D^2 \widehat{M}_X$ is integral. If the eigenvalues of A are simple then $D\widehat{M}_X$ is integral.

The End(s)