Problems with Continuous Quantum Walks

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Outline

1. Overview
   - Some History
   - Some Theory
2. Questions
   - Perfect state transfer
   - Cospectrality
   - Averaging
   - Mixing

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Collaborators: A Partial List

- Krystal Guo: CRM Montréal.
- Gabriel Coutinho: UFMG, Belo Horizonte.
- Hanmeng Zhan: York.
- Tino Tamon: Clarkson.
- Simone Severini: Amazon.
- Natalie Mullin.
- Jamie Smith: Google.

Bibliography

- Sugato Bose. Quantum Communication Through an Unmodulated Spin Chain. https://arxiv.org/abs/quant-ph/0212041
- Matthias Christandl, Nilanjana Datta, Tony C. Dorlas, Artur Ekert, Alastair Kay, Andrew J. Landahl. Perfect Transfer of Arbitrary States in Quantum Spin Networks. https://arxiv.org/abs/quant-ph/0411020
- Nitin Saxena, Simone Severini, Igor Shparlinski. Parameters of Integral Circulant Graphs and Periodic Quantum Dynamics. https://arxiv.org/abs/quant-ph/0703236

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Continuous Walks

Given a graph X with adjacency matrix A, we define transition operators $U(t)$ by

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

If we have an initial state given by a density matrix D, the state of the system at time t will be $U(t)DU(-t)$.

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Usually the initial state has the form $e_a e_a^T = |a\rangle\langle a|$ for some vertex a, and we measure in the standard basis at time t.

The Mixing Matrix

For a continuous quantum walk with transition matrix $U(t)$, the result of any measurement at time is determined by the entries of the mixing matrix $M(t)$, defined by

$$M(t) := U(t) \circ \overline{U(t)} = U(t) \circ U(-t).$$

An Example

If we take our graph to be K_2, with adjacency matrix

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

then

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

and

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

Three Cases

$$U(\pi/4) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \qquad \text{[uniform mixing]}$$

$$U(\pi/2) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}. \qquad \text{[perfect state transfer]}$$

$$U(\pi) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad \text{[periodicity]}$$

Products

Definition

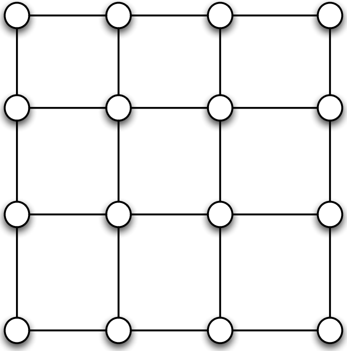
The vertex set of the Cartesian product $X \,\square\, Y$ is $V(X) \times V(Y)$, where

$$(x_1, y_1) \sim (x_2, y_2)$$

if

- $x_1 = x_2$ and $y_1 \sim y_2$, or
- $x_1 \sim x_2$ and $y_1 = y_2$.

$P_4 \square P_4$



The transition matrix of a Cartesian product

If X and Y are graphs, then

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

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The d-dimensional hypercube Q_d is the Cartesian product of d copies of K_2, whence

$$U_{Q_d}(t) = U_{K_2}(t)^{\otimes d}.$$

A consequence of this that at, times $\pi/4$, $\pi/2$ and π, we have respectively uniform mixing, perfect state transfer and periodicity on Q_d.

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Phase factors

Suppose we have perfect state transfer at time t from vertex a to vertex b in X. Then there is a complex number γ of norm one, such that

$$U(t)|a\rangle = \gamma|b\rangle.$$

Question

Must the phase factor γ be a root of unity?

In all known cases, it is.

PST on trees?

Theorem

For a fixed integer k, there are only finitely many connected graphs with maximum valency k on which perfect state transfer occurs.

I would like to replace “maximum valency k” by something like “average valency k”. The average valency of a tree is less than two.

Question

Is the a tree with more than three vertices on which perfect state transfer occurs.

Easier question on trees?

Question

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Is there a positive integer d such that no tree of diameter greater than d admits perfect state transfer?

Question

Is it true that, for a positive real c, there are only finitely many connected graphs, with average valency at most c, on which perfect state transfer takes place?

Laplacians

Let Δ be the diagonal matrix with $\Delta_{i,i}$ equal to the valency of the i-th vertex of X. The Laplacian of X is the matrix $\Delta - A$. We can use the Laplacian as the Hamiltonian for a continuous quantum walk, i.e., take

$$U(t) = \exp(it(\Delta - A)).$$

Generally using the Laplacian in place of the adjacency matrix has very little qualitative effect.

No Laplacian PST on trees

Theorem (Coutinho, Liu)

If T is a tree on at least three vertices, the continuous walk with Hamiltonian $\Delta - A$ does not admit perfect state transfer.

See Coutinho, Liu: "No Laplacian perfect state transfer in trees"
`https://arxiv.org/abs/1408.2935`

Outline

Symmetry and Periodicity

Asssume $a, b \in V(X)$ and we have perfect state transfer from a to b at time t. Then there is a complex scalar γ of norm one such that $U(t)|a\rangle = \gamma|b\rangle$. Taking complex conjugates and noting that $|a\rangle$ and $|b\rangle$ are real, we get

$$U(-t)|a\rangle = \gamma^{-1}|b\rangle$$

and consequently

$$\gamma|a\rangle = U(t)|b\rangle$$

We note that

$$\gamma^{-1}U(t)|a\rangle = |b\rangle, \qquad \gamma^{-1}U(t)|b\rangle = |a\rangle$$

An example: cospectral vertices

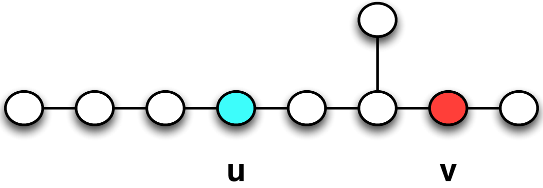


Figure: Schwenk's Tree, 1973

$$\phi(T \setminus u, t) = \phi(T \setminus v, t)$$

Cospectrality and Symmetry

Theorem

Vertices a and b in the graph X are cospectral if and only if there is an orthogonal matrix Q such that

1. *Q commutes with A.*
2. *$Q|a\rangle = |b\rangle$.*
3. *$Q^2 = I$.*

Taking $Q = \gamma^{-1}U(t)$, we see that if we have perfect state transfer from a to b, then a and b are cospectral.

Strongly cospectral vertices

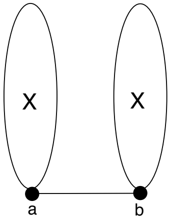
Definition

Vertices a and b in the graph X are cospectral if and only if there is an orthogonal matrix Q such that

1. Q commutes with A.
2. $Q|a\rangle = |b\rangle$.
3. $Q^2 = I$.
4. Q is a polynomial in A.

Vertices related by perfect state transfer must be strongly cospectral. If the eigenvalues of A are simple, cospectral vertices are strongly cospectral. (For more on strongly cospectral vertices see Godsil and Smith "Strongly cospectral vertices".) `https://arxiv.org/abs/1709.07975v1`.

A possibility for perfect state transfer



The vertices a and b in this graph are strongly cospectral.

Question

If there a connected graph X with more than one vertex, such that there is perfect state transfer between vertices a and b in the graph above?

Orbits

If $u \in V(X)$, define D_u to be the density matrix $|u\rangle\langle u|$. Note that

$$\Gamma = \{U(t) : t \in \mathbb{R}\}$$

is a group and the set

$$\{U(t)D_aU(-t) : t \in \mathbb{R}\}$$

is the orbit of D_a under the action of Γ. Hence we have perfect state transfer from a to b if and only if D_b lies in the Γ-orbit of D_a.

Pretty good state transfer

Definition

We have pretty good state transfer from a to b if D_b lies in the closure of the orbit of D_a.

More prosaically, we have pretty good state transfer if, for each $\psi > 0$ there is a time t such that $\|U(t)D_aU(-t) - D_b\| < \epsilon$.

PGST and Number Theory

Theorem (Godsil, Kirkland, Severini, Smith)

We have pretty good state transfer between the end-vertices of the path P_n (on n vertices) if and only if one the following holds:

a. $n+1$ *is a power of* 2.
b. $n+1$ *is a prime number.*
c. $n+1$ *is twice a prime number.*

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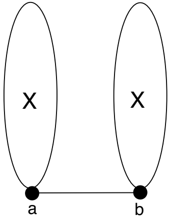
(The only paths with perfect state transfer between their end-vertices are P_2 and P_3.)

Possibilities for pretty good state transfer



Question

For which connected graphs X do we have pretty good state transfer between vertices a and b in the graph above?

Examples

Theorem

If X is the star $K_{1,m}$, then graph produced by the previous construction admits pretty good state transfer between the central vertices if and only if $4m+1$ is a perfect square.

See Xiaoxia Fan, Chris Godsil. “Pretty good state transfer on double stars” https://arxiv.org/abs/1206.0082v3

How hard is it?

We can determine in polynomial time whether a graph admits perfect state transfer. (Coutinho, Godsil "Perfect state transfer is poly-time", `https://arxiv.org/abs/1606.02264v1`). Coutinho asks:

Question

Is it possible to determine in polynomial time whether a graph admits pretty good state transfer?

Outline

A new invariant

Recall the mixing matrix $M(t) = U(t) \circ U(-t)$.

Definition

The average mixing matrix $\widehat{M}$ is defined by

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

(For more, see Godsil "Average mixing matrices of continuous quantum walks" `https://arxiv.org/abs/1103.2578v3`.)

Expressions for $M(t)$ and $\widehat{M}$

If the adjacency matrix A of X has the spectral decomposition $A = \sum_r \theta_r E_r$ then we also have $U(t) = \sum_r e^{it\theta_r} E_r$ and so

$$M(t) = U(t) \circ U(-t) = \sum_{r,s} e^{it(\theta_r - \theta_s)} E_r \circ E_s.$$

Now some elementary calculus implies that

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

The complete graphs

The idempotents in the spectral decomposition of K_n are

$$\frac{1}{n}J, \quad I - \frac{1}{n}J$$

and therefore

$$\widehat{M}_{K_n} = \Big(1 - \frac{2}{n}\Big)I + \frac{1}{n^2}J,$$

with the surprising consequence that, for large n,

$$\widehat{M}_{K_n} \approx I.$$

Properties of $\widehat{M}$

The average mixing matrix has a number of interesting properties:

a. It is positive semidefinite.
b. Its entries are rational.
c. Two rows are equal if and only if the corresponding vertices are strongly cospectral.

Rank of $\widehat{M}$

We know that if $\mathrm{rk}(\widehat{M}) = 1$, then X has at most two vertices.

Question

Are there infinitely many graphs X such that $\mathrm{rk}(\widehat{M}) = 2$?

Theorem

We have

$$I \succcurlyeq M(t) \succcurlyeq 2\widehat{M} - I.$$

For the complete graph, this yields

$$I \succcurlyeq M(t) \succcurlyeq \Big(1 - \frac{4}{n}\Big) I + \frac{2}{n^2} J.$$

and thus the diagonal entries of $M(t)$ are bounded below by

$$1 - \frac{4}{n} + \frac{2}{n^2}.$$

Sedentary walks

Definition

A family of graphs is sedentary if there is a constant c such that the probability a continuous quantum walk is on its initial vertex is at least $1 - \frac{c}{n}$, at any time.

Thus complete graphs are sedentary.

Question

Is there a sedentary family of connected cubic graphs?

Outline

Uniform mixing, local uniform mixing

Definition

We have uniform mixing on a walk on X if there is a time t such that

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

if all entries of the a-row of $M(t)$ are equal (necessarily to $1/|V(X)|$), we have local uniform mixing at a.

What we know about uniform mixing

- K_2 admits uniform mixing at time $\pi/4$, and so
- The hypercube also admits uniform mixing at time $\pi/4$.
- There are many cases where we have perfect state transfer at time t and uniform mixing at time $t/2$.
- The complete bipartite graph $K_{1,3}$ (and its Cartesian powers) admit uniform mixing. [H. Zhan]
- The only even cycle that admits uniform mixing is C_4, the only cycle of prime length that admits uniform mixing is K_3. [N. Mullin]
- The stars $K_{1,n}$ admit local uniform mixing at their central vertex.

What we don't know

Questions

- Which odd cycles admit uniform mixing?
- Is there a graph other than $K_{1,3}$ that is not regular and admits uniform mixing?
- Which trees admit local uniform mixing?

More of what we don't know

Two conjectures due to N. Mullin.

Conjectures

- If a graph admits uniform mixing at time t, then e^{it} is a root of unity.
- If $n \geq 5$, no connected Cayley graph for $\mathbb{Z}_n^d$ admits uniform mixing.

There are families of Cayley graphs for $\mathbb{Z}_2^d$ and $\mathbb{Z}_3^d$ that do admit uniform mixing. [A. Chan, N. Mullin, H. Zhan]
More information in Godsil, Mullin, Roy "Uniform mixing and association schemes" `https://www.combinatorics.org/ojs/index.php/eljc/article/view/v24i3p22`.

The End(s)