Continuous quantum walks

Arnbjörg Soffía Árnadóttir

Faculty of Mathematics
University of Waterloo

August, 2019

UNIVERSITY OF WATERLOO

Outline

UNIVERSITY OF WATERLOO

Random Walks

Definition 1

Let X be a graph. Its *adjacency matrix*, $A = A(X)$, is indexed by $V(X)$ and is defined by

$$A_{u,v} = \begin{cases} 1 & \text{if } u \sim v, \\ 0 & \text{otherwise.} \end{cases}$$

The *degree matrix*, Δ, of X is the diagonal matrix with $\Delta_{u,u} = \deg(u)$. The *Laplacian* of X is the matrix $L = \Delta - A$.

Random Walks

Definition 2

Let X be a graph with adjacency matrix A, degree matrix Δ and Laplacian $L = \Delta - A$. The *continuous random walk* on X is given by

$$M(t) = e^{-tL} = \sum_{n\geq 0} \frac{(-t)^n}{n!} L^n, \quad t \in [0, \infty).$$

Quantum Walks

Definition 3

Let H be a real symmetric matrix. The *continuous quantum walk* on H is given by the matrix

$$U(t) := e^{itH} = \sum_{n \geq 0} \frac{(it)^n}{n!} H^n, \quad t \in \mathbb{R}.$$

The matrix $U(t)$ is called the *transition matrix* of the walk.

$U(t)$ is a unitary matrix for all t.

Quantum Walks

Definition 3

Let H be a real symmetric matrix. The *continuous quantum walk* on H is given by the matrix

$$U(t) := e^{itH} = \sum_{n \geq 0} \frac{(it)^n}{n!} H^n, \quad t \in \mathbb{R}.$$

The matrix $U(t)$ is called the *transition matrix* of the walk.

$U(t)$ is a unitary matrix for all t.

Mixing matrix

Definition 4

Given a continuous quantum walk with transition matrix $U(t)$, we define the *mixing matrix* of the walk by

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

Since $U(t)$ is unitary the norm of each row is one, and so $M(t)$ is a stochastic matrix for all t.

Mixing matrix

Definition 4

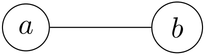
Given a continuous quantum walk with transition matrix $U(t)$, we define the *mixing matrix* of the walk by

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

Since $U(t)$ is unitary the norm of each row is one, and so $M(t)$ is a stochastic matrix for all t.

UNIVERSITY OF WATERLOO

Example - K_2



K_2

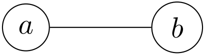
We have

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{so} \quad A^{2n} = I, \text{ and } A^{2n+1} = A,$$

for all n. Therefore

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

Example - K_2



K_2

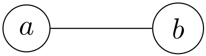
We have

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{so} \quad A^{2n} = I, \text{ and } A^{2n+1} = A,$$

for all n. Therefore

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

Example - K_2



K_2

We have

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{so} \quad A^{2n} = I, \text{ and } A^{2n+1} = A,$$

for all n. Therefore

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

Example - K_2

So the transition matrix at time t is

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

and the mixing matrix

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

Perfect State Transfer

Definition 5

For distinct vertices, u and v of X, we say that we have *perfect state transfer (pst)* from u to v at time t if

$$U(t)e_u = \gamma e_v,$$

for some scalar γ with $|\gamma| = 1$ or, equivalently, if

$$M(t)_{u,v} = 1.$$

Periodicity

Definition 6

We say that a vertex u is *periodic* at time t if

$$U(t)e_u = \gamma e_u,$$

for some scalar γ with $|\gamma| = 1$ or, equivalently, if

$$M(t)_{u,u} = 1.$$

We say that a graph X is periodic at time t if $U(t)$ is diagonal.

Uniform mixing

Definition 7

We say that we have *uniform mixing* at time t if all entries of $U(t)$ have the same absolute value or, equivalently, if all entries of $M(t)$ are equal.

Example - K_2 (continued)

Recall that for K_2,

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

We see that

$$U(\pi/4) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad U(\pi/2) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \text{and} \quad U(\pi) = -I.$$

Example - K_2 (continued)

Recall that for K_2,

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

We see that

$$U(\pi/4) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad U(\pi/2) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \text{and} \quad U(\pi) = -I.$$

Theorem 8

If there is perfect state transfer from u to v at time t, then there is perfect state transfer from v to u at time t. It follows that u and v are periodic at time $2t$.

Theorem 9 (Kay, 2011)

If there is perfect state transfer from u to v in X and from u to w, then $v = w$.

Theorem 8

If there is perfect state transfer from u to v at time t, then there is perfect state transfer from v to u at time t. It follows that u and v are periodic at time $2t$.

Theorem 9 (Kay, 2011)

If there is perfect state transfer from u to v in X and from u to w, then $v = w$.

Spectral decomposition

Let A be a hermitian matrix with distinct eigenvalues, $\theta_0, \theta_1, \ldots, \theta_d$. Then A can be written as

$$A = \sum_{r=0}^{d} \theta_r E_r$$

where the matrices E_r satisfy

- $E_r^2 = E_r$
- $E_r E_s = 0$, if $r \neq s$
- $\sum_r E_r = I$.

This is called the *spectral decomposition* of A.

UNIVERSITY OF WATERLOO

Spectral decomposition

Theorem 10

If A is a hermitian matrix with distinct eigenvalues $\theta_0, \ldots, \theta_d$, and f is a univariate function whose Taylor series converges to f on the spectrum of A, then

$$f(A) = \sum_{r=0}^{d} f(\theta_r) E_r.$$

It follows that if A is the adjacency matrix of a graph then

$$U(t) = e^{itA} = \sum_{r=0}^{d} e^{it\theta_r} E_r.$$

UNIVERSITY OF WATERLOO

Spectral decomposition

Theorem 10

If A is a hermitian matrix with distinct eigenvalues $\theta_0, \dots, \theta_d$, and f is a univariate function whose Taylor series converges to f on the spectrum of A, then

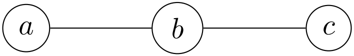
$$f(A) = \sum_{r=0}^{d} f(\theta_r) E_r.$$

It follows that if A is the adjacency matrix of a graph then

$$U(t) = e^{itA} = \sum_{r=0}^{d} e^{it\theta_r} E_r.$$

UNIVERSITY OF WATERLOO

Example - P_3



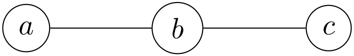
P_3

The adjacency matrix has eigenvalues $\sqrt{2}, 0, -\sqrt{2}$, and spectral idempotents (respectively)

$$E_0 = \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}, \quad E_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

$$E_2 = \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}.$$

Example - P_3



P_3

The adjacency matrix has eigenvalues $\sqrt{2}, 0, -\sqrt{2}$, and spectral idempotents (respectively)

$$E_0 = \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}, \quad E_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

$$E_2 = \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}.$$

Example - P_3

Therefore

$$U(t) = e^{it\sqrt{2}}E_0 + E_1 + e^{-it\sqrt{2}}E_2$$

and so

$$U(\pi/\sqrt{2}) = -E_0 + E_1 - E_2 = -\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

We see that we have pst between a and c at time $\pi/\sqrt{2}$ and b is periodic at that time.

Example - P_3

Therefore

$$U(t) = e^{it\sqrt{2}}E_0 + E_1 + e^{-it\sqrt{2}}E_2$$

and so

$$U(\pi/\sqrt{2}) = -E_0 + E_1 - E_2 = -\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

We see that we have pst between a and c at time $\pi/\sqrt{2}$ and b is periodic at that time.

Paths

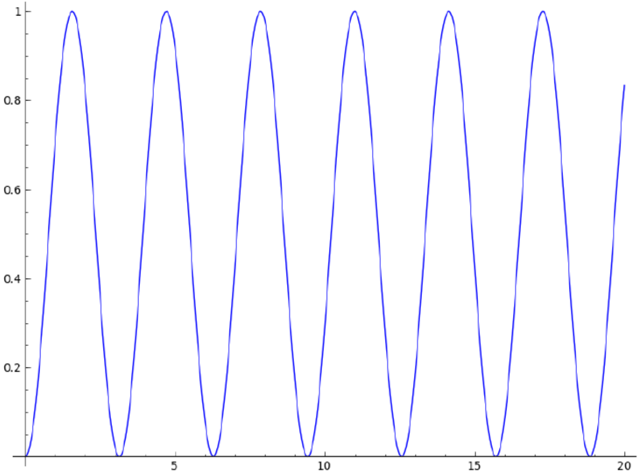


Figure: $P_2 : M(t)_{0,1}$

Paths

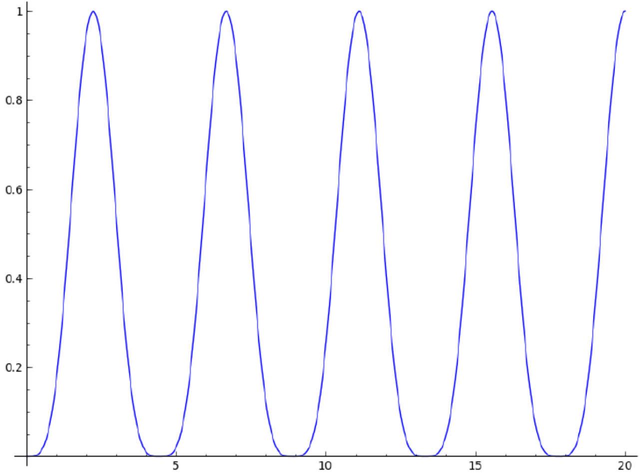


Figure: $P_3 : M(t)_{0,2}$

Paths

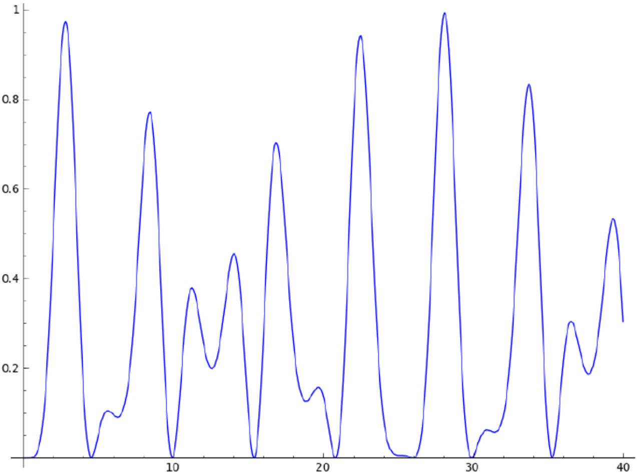


Figure: $P_4 : M(t)_{0,3}$

Complete graphs

The complete graph on n vertices has adjacency matrix $J - I$.
It has eigenvalues $n - 1$, and -1 and the corresponding spectral idempotents are

$$E_0 := \frac{1}{n} J, \qquad E_1 := I - \frac{1}{n} J.$$

Therefore

$$U(t) = e^{it(n-1)} E_0 + e^{-it} E_1 = e^{-it} \left(I + \frac{e^{itn} - 1}{n} J \right)$$

Complete graphs

The complete graph on n vertices has adjacency matrix $J - I$. It has eigenvalues $n-1$, and -1 and the corresponding spectral idempotents are

$$E_0 := \frac{1}{n} J, \qquad E_1 := I - \frac{1}{n} J.$$

Therefore

$$U(t) = e^{it(n-1)} E_0 + e^{-it} E_1 = e^{-it} \left(I + \frac{e^{itn} - 1}{n} J \right)$$

Complete graphs

The complete graph on n vertices has adjacency matrix $J - I$. It has eigenvalues $n-1$, and -1 and the corresponding spectral idempotents are

$$E_0 := \frac{1}{n} J, \qquad E_1 := I - \frac{1}{n} J.$$

Therefore

$$U(t) = e^{it(n-1)} E_0 + e^{-it} E_1 = e^{-it} \left(I + \frac{e^{itn} - 1}{n} J \right)$$

Complete graphs

For any vertex u and any time t we have

$$U(t)_{u,u} = e^{-it}\left(1 + \frac{e^{itn} - 1}{n}\right)$$

and so

$$|U(t)_{u,u}| \geq 1 - \frac{2}{n}.$$

Cayley graphs

Definition 11

Let G be a group and $\mathcal{C} \subseteq G \backslash e$ a subset with $\mathcal{C}^{-1} = \mathcal{C}$. The *Cayley graph*, $X := X(G, \mathcal{C})$, has vertex set $V(X) := G$ and

$$g \sim h \quad \text{if} \quad hg^{-1} \in \mathcal{C}.$$

UNIVERSITY OF WATERLOO

Cayley graphs

A group acts transitively on itself by right/left multiplication.
It follows that

- Cayley graphs are vertex transitive,
- the adjacency matrix of a Cayley graph can be written as

$$A = P_1 + \cdots + P_k$$

where $k = |\mathcal{C}|$ and P_i are permutation matrices.

Cayley graphs

A group acts transitively on itself by right/left multiplication. It follows that

- Cayley graphs are vertex transitive,
- the adjacency matrix of a Cayley graph can be written as

$$A = P_1 + \cdots + P_k$$

where $k = |C|$ and P_i are permutation matrices.

UNIVERSITY OF WATERLOO

Cayley graphs

A group acts transitively on itself by right/left multiplication. It follows that

- Cayley graphs are vertex transitive,
- the adjacency matrix of a Cayley graph can be written as

$$A = P_1 + \cdots + P_k$$

where $k = |\mathcal{C}|$ and P_i are permutation matrices.

Vertex transitive graphs

Theorem 12 (Godsil, 2010)

Let X be a vertex transitive graph, and suppose there is perfect state transfer from u to v at time t. Then there is some scalar γ and some permutation matrix P with order two such that

$$U(t) = \gamma P.$$

Moreover, P is an automorphism of X that has no fixed points.

Cubelike graphs

Definition 13

A *cubelike graph* is a Cayley graph of the elementary abelian group $\mathbb{Z}_2^n$.

Theorem 14 (Bernasconi et al., 2008)

Let $X = X(\mathbb{Z}_2^n, \mathcal{C})$ be a cubelike graph. Then X is periodic with period dividing π. Its period is equal to π if and only if

$$c := \sum_{g \in \mathcal{C}} g \neq 0$$

and in this case there is perfect state transfer from 0 to c at time $\pi/2$.

Cubelike graphs

Definition 13

A *cubelike graph* is a Cayley graph of the elementary abelian group $\mathbb{Z}_2^n$.

Theorem 14 (Bernasconi et al., 2008)

Let $X = X(\mathbb{Z}_2^n, \mathcal{C})$ be a cubelike graph. Then X is periodic with period dividing π. Its period is equal to π if and only if

$$c := \sum_{g \in \mathcal{C}} g \neq 0$$

and in this case there is perfect state transfer from 0 to c at time $\pi/2$.

Proof.

We can write $A = A(X)$ as a sum of permutation matrices

$$A = P_1 + \cdots + P_k, \qquad P_r^2 = I, \quad P_r P_s = P_s P_r.$$

Then

$$e^{itA} = e^{it(P_1 + \cdots + P_k)} = \prod_{r=1}^{k} e^{itP_r}.$$

Also, $e^{itP_r} = \cos(t)I + i\sin(t)P_r$, so

$$U(t) = \prod_{r=1}^{k} \left(\cos(t)I + i\sin(t)P_r\right),$$

thus $U(\pi/2) = i^k \prod_r P_r$. □

Proof.

We can write $A = A(X)$ as a sum of permutation matrices

$$A = P_1 + \cdots + P_k, \qquad P_r^2 = I, \quad P_r P_s = P_s P_r.$$

Then

$$e^{itA} = e^{it(P_1 + \cdots + P_k)} = \prod_{r=1}^{k} e^{itP_r}.$$

Also, $e^{itP_r} = \cos(t)I + i\sin(t)P_r$, so

$$U(t) = \prod_{r=1}^{k} \left(\cos(t)I + i\sin(t)P_r\right),$$

thus $U(\pi/2) = i^k \prod_r P_r$. $\square$

Proof.

We can write $A = A(X)$ as a sum of permutation matrices

$$A = P_1 + \cdots + P_k, \qquad P_r^2 = I, \quad P_r P_s = P_s P_r.$$

Then

$$e^{itA} = e^{it(P_1 + \cdots + P_k)} = \prod_{r=1}^{k} e^{itP_r}.$$

Also, $e^{itP_r} = \cos(t)I + i\sin(t)P_r$, so

$$U(t) = \prod_{r=1}^{k} \left(\cos(t)I + i\sin(t)P_r\right),$$

thus $U(\pi/2) = i^k \prod_r P_r$. □

Thank you

Cayley graphs of S_n

Theorem 15 (Gerhardt, Watrous; 2003)

Let $X = X(S_n, \mathcal{C})$ where $\mathcal{C}$ is the set of transpositions of S_n and let $M(t)$ be the mixing matrix of a continuous quantum walk on X. If σ is any n-cycle of S_n, then

$$M(t)_{e,\sigma} \leq \frac{2^{2n-2}}{(n!)^2}.$$

UNIVERSITY OF WATERLOO

Paths

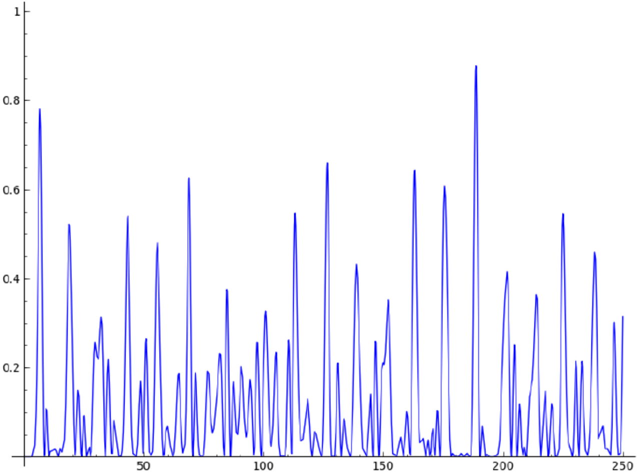


Figure: $P_{11} : M(t)_{0,10}$