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Time averaged distributions for CTQWs and DTQWs on the path

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Abstract—In this talk, we will focus on the time averaged distributions for continuous-time quantum walks (CTQWs) and Szegedy's walk a type of discrete-time quantum walks (DTQWs) on the path graph induced by the birth and death chain (discrete-time random walk with reflecting walls) on it.

1. Introduction

The study of quantum walks, known as quantum counterparts of random walks, has been extensively developed in various fields during the last 20 years. There are good review articles for these developments such as Kempe [5], Kendon [6], Venegas-Andraca [13, 14], Konno [7], Manouchehri and Wang [8], and Portugal [10].

In this talk, we will focus on the time averaged distribution of a variant of discrete time quantum walk (DTQW) so-called Szegedy's walk [12]. On the path graph, the spectral properties of Szegedy's walk are directly connected to the theory of (finite type) orthogonal polynomials. There are studies of the distribution of Szegedy's walk on the path graph for example [2,4,9,11].

2. Definition of the models

In order to define our models, we consider the path graph $P_{n+1} = (V(P_{n+1}), E(P_{n+1}))$ with the vertex set $V(P_{n+1}) = \{0, 1, \ldots, n\}$ and the (undirected) edge set $E(P_{n+1}) = \{(j, j+1) : j = 0, 1, \ldots, n-1\}$. On the path graph P_{n+1}, we define a discrete time random walk (DTRW) with reflecting walls as follows:

Let p_j^L be the transition probability of the random walker at the vertex $j \in V(P_{n+1})$ to the left $(j-1 \in V(P_{n+1}))$. Also let $p_j^R = 1 - p_j^L$ be the transition probability of the random walker at the vertex $j \in V(P_{n+1})$ to the right $(j+1 \in V(P_{n+1}))$. For the sake of simplicity, we assume $0 < p_j^L, p_j^R < 1$ except for $j = 0, n$. We put the reflecting walls at the vertex $0 \in V(P_{n+1})$ and the vertex $n \in V(P_{n+1})$, i.e., we set $p_0^R = p_n^L = 1$. We also call this type of DTRW as the birth and death chain.

We define a positive constant C_π as

$$C_\pi := 1 + \sum_{j=1}^{n} \frac{p_0^R \cdot p_1^R \cdots p_{j-1}^R}{p_1^L \cdot p_2^L \cdots p_j^L}.$$

By using this constant, we can define the stationary distribution $\{\pi(0), \pi(1), \ldots, \pi(n)\}$ as

$$\pi(j) = \begin{cases} \frac{1}{C_\pi} & \text{if } j = 0, \\ \frac{1}{C_\pi} \cdot \frac{p_0^R \cdot p_1^R \cdots p_{j-1}^R}{p_1^L \cdot p_2^L \cdots p_j^L} & \text{if } j = 1, 2, \ldots, n. \end{cases}$$

Note that $\pi(j) > 0$ for all $j \in V(P_{n+1})$ and the stationary distribution is satisfied with so-called the detailed balance condition,

$$\pi(j) \cdot p_j^R = p_{j+1}^L \cdot \pi(j+1),$$

for $j = 0, 1, \ldots n-1$.

In order to define a continuous time quantum walk (CTQW) corresponding to the DTRW, we introduce the normalized Laplacian matrix $\mathcal{L}$. Let P be the transition matrix of the DTRW. Also we define diagonal matrices $D_\pi^{1/2} := \mathrm{diag}\left(\sqrt{\pi(0)}, \sqrt{\pi(1)}, \ldots, \sqrt{\pi(n)}\right)$ and $D_\pi^{-1/2} = \mathrm{diag}\left(1/\sqrt{\pi(0)}, 1/\sqrt{\pi(1)}, \ldots, 1/\sqrt{\pi(n)}\right)$. The normalized Laplacian matrix $\mathcal{L}$ is given by

$$\mathcal{L} := D_\pi^{1/2} (I_{n+1} - P) D_\pi^{-1/2} = I_{n+1} - D_\pi^{1/2} P D_\pi^{-1/2},$$

where I_{n+1} be the $(n+1)\times(n+1)$ identity matrix. We should remark that the matrix

$$J := D_\pi^{1/2} P D_\pi^{-1/2},$$

is referred as the Jacobi matrix. So we can rewrite $\mathcal{L}$ as $\mathcal{L} = I_{n+1} - J$.

By using the detailed balance condition, we obtain

$$J_{j,k} = J_{k,j} = \begin{cases} \sqrt{p_j^L p_{j+1}^R}, & \text{if } k = j+1, \\ 0, & \text{otherwise.} \end{cases}$$

Thus $\mathcal{L} = I_{n+1} - J$ is an Hermitian matrix (real symmetric matrix). The CTQW which is discussed in this paper is driven by the time evolution operator (unitary matrix)

$$U_{CTQW}(t) := \exp(it\mathcal{L}) := \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \mathcal{L}^k,$$

where i is the imaginary unit. Let X_t^C $(t \geq 0)$ be the random variable representing the position of the CTQWer at time t. The distribution of X_t^C is determined by

$$\mathbb{P}\left(X_t^C = k | X_0^C = j\right) := \left|\langle k | U_{CTQW}(t) | j \rangle\right|^2 = \left|(U_{CTQW}(t))_{k,j}\right|^2,$$

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where $|j\rangle$ is the $(n+1)$-dimensional unit vector (column vector) which j-th component equals 1 and the other components are 0 and $\langle v|$ is the transpose of $|v\rangle$, i.e., $\langle v| = {}^T|v\rangle$.

Hereafter we only consider $X_0^C = 0$, i.e., the CTQWer starts from the left most vertex $0 \in V(P_{n+1})$, cases. The time averaged distribution $\bar{p}_C$ of the CTQW is defined by

$$\bar{p}_C(j) := \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathbb{P}\left(X_t^C = j | X_0^C = 0\right) dt,$$

for each vertex $j \in V(P_{n+1})$. We define a random variable $\bar{X}_n^C$ as $\mathbb{P}\left(\bar{X}_n^C = j\right) = \bar{p}_C(j)$.

In this talk, we also deal with a type of discrete time quantum walk (DTQW) corresponding to the DTRW so-called Szegedy's walk. The time evolution operator for the DTQW is defined by $U = SC$ with the coin operator C and the shift operator (flip-flop type shift) S. The coin operator C is defined by

$$C = |0\rangle\langle 0| \otimes I_2 + \sum_{j=1}^{n-1} |j\rangle\langle j| \otimes C_j + |n\rangle\langle n| \otimes I_2,$$

where I_2 is the 2×2 identity matrix and $\otimes$ is the tensor product. The local coin operator C_j is defined by

$$C_j = 2|\phi_j\rangle\langle\phi_j| - I_2, \quad |\phi_j\rangle = \sqrt{p_j^L}|L\rangle + \sqrt{p_j^R}|R\rangle,$$

where $|L\rangle = {}^T[1\ 0]$ and $|R\rangle = {}^T[0\ 1]$. The shift operator S is given by

$$S\left(|j\rangle \otimes |L\rangle\right) = |j-1\rangle \otimes |R\rangle, \quad S\left(|j\rangle \otimes |R\rangle\right) = |j+1\rangle \otimes |L\rangle.$$

Let X_t^D $(t = 0, 1, \ldots)$ be the random variable representing the position of the DTQWer at time t. In this paper, we only consider $X_0^D = 0$ cases. The distribution of X_t^D is defined by

$$\begin{aligned}\mathbb{P}\left(X_t^D = j | X_0^D = 0\right) :&= \left\|\left(\langle j| \otimes I_2\right) U_{DTQW}(t) \left(|0\rangle \otimes |R\rangle\right)\right\|^2 \\ &= \left|\left(\langle j| \otimes \langle L|\right) U_{DTQW}(t) \left(|0\rangle \otimes |R\rangle\right)\right|^2 \\ &\quad + \left|\left(\langle j| \otimes \langle R|\right) U_{DTQW}(t) \left(|0\rangle \otimes |R\rangle\right)\right|^2.\end{aligned}$$

We also consider the time averaged distribution $\bar{p}_D$ of the DTQW defined by

$$\bar{p}_D(j) := \lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} \mathbb{P}\left(X_t^D = j | X_0^D = 0\right),$$

for each vertex $j \in V(P_{n+1})$. We define a random variable $\bar{X}_n^D$ as $\mathbb{P}\left(\bar{X}_n^D = j\right) = \bar{p}_D(j)$.

3. Relations between $\bar{X}_n^C$ and $\bar{X}_n^D$

Since the Jacobi matrix J is a real symmetric matrix with simple [3] and symmetric [2] eigenvalues, we obtain eigenvalues $1 = \lambda_0 > \lambda_1 > \cdots > \lambda_{n-1} > \lambda_n = -1$ and corresponding eigenvectors $\{|v_\ell\rangle\}_{\ell=0}^n$ as an orthonormal basis of n-dimensional complex vector space $\mathbb{C}^n$. Thus we have the spectral decomposition

$$J = \sum_{\ell=0}^{n} \lambda_\ell |v_\ell\rangle\langle v_\ell|.$$

Noting that $\mathcal{L} = I_{n+1} - J$, the spectral decomposition of $U_{CTQW}(t)$ is given by

$$\begin{aligned}U_{CTQW}(t) &= \sum_{\ell=0}^{n} \exp\left[it\left(1-\lambda_\ell\right)\right] |v_\ell\rangle\langle v_\ell| \\ &= e^{it} \sum_{\ell=0}^{n} e^{-it\lambda_\ell} |v_\ell\rangle\langle v_\ell|.\end{aligned}$$

Because of simple eigenvalues of the Jacobi matrix J, the time averaged distribution $\bar{p}_C$ is expressed by

$$\bar{p}_C(j) = \sum_{\ell=0}^{n} |\langle j|v_\ell\rangle|^2 \, |\langle v_\ell|0\rangle|^2 = \sum_{\ell=0}^{n} |v_\ell(j)|^2 \, |v_\ell(0)|^2,$$

where $v_\ell(j)$ is the jth component of $|v_\ell\rangle$.

On the other hand, the spectral decomposition of $U_{DTQW}(t)$ is given (see e.g. [2, 4, 11, 12]) by

$$\begin{aligned}U_{DTQW}(t) &= \mu_0 |u_0\rangle\langle u_0| \\ &\quad + \sum_{\ell=1}^{n-1} \left(\frac{1}{2(1-\lambda_\ell^2)} \sum_{\pm} \mu_{\pm\ell} |u_{\pm\ell}\rangle\langle u_{\pm\ell}| \right) \\ &\quad + \mu_n |u_n\rangle\langle u_n|,\end{aligned}$$

where

$$\begin{cases}\mu_0 = \lambda_0 = 1, & |u_0\rangle = |\overline{v_0}\rangle, \\ \mu_{\pm\ell} = \exp\left(\pm i \cos^{-1}\lambda_\ell\right), & |u_{\pm\ell}\rangle = |\overline{v_\ell}\rangle - \mu_{\pm\ell}\, S|\overline{v_\ell}\rangle, \\ \mu_n = \lambda_n = -1, & |u_{n-1}\rangle = |\overline{v_{n-1}}\rangle,\end{cases}$$

with

$$|\overline{v_\ell}\rangle = v_\ell(0)|0\rangle \otimes |R\rangle + \sum_{j=1}^{n-1} v_\ell(j)|j\rangle \otimes |\phi_j\rangle + v_\ell(n)|n\rangle \otimes |L\rangle.$$

All the eigenvalues of $U_{DTQW}(t)$ are also simple, the time averaged distribution $\bar{p}_D$ is expressed by

$$\begin{aligned}\bar{p}_D(j) &= \left\{ |(\langle j| \otimes \langle L|)\,|u_0\rangle|^2 + |(\langle j| \otimes \langle R|)\,|u_0\rangle|^2 \right\} |\langle u_0|\,(|0\rangle \otimes |R\rangle)|^2 \\ &\quad + \sum_{\ell=1}^{n-1} \left[\frac{1}{2(1-\lambda_\ell^2)} \sum_{\pm} \left\{ |(\langle j| \otimes \langle L|)\,|u_{\pm\ell}\rangle|^2 \right.\right. \\ &\qquad \left.\left. + |(\langle j| \otimes \langle R|)\,|u_{\pm\ell}\rangle|^2 \right\} |\langle u_{\pm\ell}|\,(|0\rangle \otimes |R\rangle)|^2 \right] \\ &\quad + \left\{ |(\langle j| \otimes \langle L|)\,|u_n\rangle|^2 + |(\langle j| \otimes \langle R|)\,|u_n\rangle|^2 \right\} |\langle u_n|\,(|0\rangle \otimes |R\rangle)|^2.\end{aligned}$$

More concrete expression of $\bar{p}_D$ in terms of eigenvalues and eigenvectors of the Jacobi matrix J is given as follows (rearrangement of Eq.(10) in [2]):

$$\bar{p}_D(j) = \frac{1}{2}|v_0(j)|^2|v_0(0)|^2 + \frac{1}{2}|v_n(j)|^2|v_n(0)|^2 + \frac{1}{2}\sum_{\ell=0}^{n}|v_\ell(j)|^2|v_\ell(0)|^2 + \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}\left\{p_{j-1}^R|v_\ell(j-1)|^2 - \lambda_\ell^2|v_\ell(j)|^2 + p_{j+1}^L|v_\ell(j+1)|^2\right\}|v_\ell(0)|^2,$$

with conventions $p_{-1}^R = v_\ell(-1) = p_{n+1}^L = v_\ell(n+1) = 0$.

Now we consider the distribution functions $\bar{F}_n^C(x) := \mathbb{P}\left(\bar{X}_n^C \le x\right) = \sum_{j\le x}\bar{p}_C(j)$ of $\bar{X}_n^C$ and $\bar{F}_n^D(x) := \mathbb{P}\left(\bar{X}_n^D \le x\right) = \sum_{j\le x}\bar{p}_D(j)$ of $\bar{X}_n^D$. For each integer $0 \le k \le n-1$, we have

$$\bar{F}_n^C(k) = \sum_{j=0}^{k}\bar{p}_C(j) = \sum_{j=0}^{k}\left\{\sum_{\ell=0}^{n}|v_\ell(j)|^2|v_\ell(0)|^2\right\}.$$

We also obtain the following expression by using $p_j^L + p_j^R = 1, p_0^R = 1$ and $p_1^L|v_\ell(1)|^2 = \lambda_\ell^2|v_\ell(0)|^2$:

$$\begin{aligned}
\bar{F}_n^D(k) &= \sum_{j=0}^{k}\bar{p}_D(j)\\
&= \frac{1}{2}\sum_{j=0}^{k}|v_0(j)|^2|v_0(0)|^2 + \frac{1}{2}\sum_{j=0}^{k}|v_n(j)|^2|v_n(0)|^2\\
&+ \frac{1}{2}\sum_{j=0}^{k}\left\{\sum_{\ell=0}^{n}|v_\ell(j)|^2|v_\ell(0)|^2\right\}\\
&+ \frac{1}{2}\sum_{j=1}^{k}\left\{\sum_{\ell=1}^{n-1}|v_\ell(j)|^2|v_\ell(0)|^2\right\}\\
&+ \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}\left\{p_0^R|v_\ell(0)|^2 - p_1^L|v_\ell(1)|^2 - p_k^R|v_\ell(k)|^2 + p_{k+1}^L|v_\ell(k+1)|^2\right\}|v_\ell(0)|^2\\
&= \sum_{j=0}^{k}\left\{\sum_{\ell=0}^{n}|v_\ell(j)|^2|v_\ell(0)|^2\right\}\\
&+ \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}\left\{-p_k^R|v_\ell(k)|^2 + p_{k+1}^L|v_\ell(k+1)|^2\right\}|v_\ell(0)|^2\\
&= \bar{F}_n^C(k)\\
&+ \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}\left\{-p_k^R|v_\ell(k)|^2 + p_{k+1}^L|v_\ell(k+1)|^2\right\}|v_\ell(0)|^2.
\end{aligned}$$

4. Scaling limit

Let $\bar{F}$ be the distribution function of the random variable $\bar{X}$. We assume that

$$\lim_{n\to\infty}\mathbb{P}\left(\frac{\bar{X}_n^C}{n} \le x\right) = \bar{F}(x) \quad (1)$$

for all points x at which $\bar{F}$ is continuous. Hereafter we assume $\bar{F}$ is continuous at x $(0 \le x \le 1)$. Remark that from the definition, Eq. (1) means that

$$\lim_{n\to\infty}\bar{F}_n^C(nx) = \lim_{n\to\infty}\bar{F}_n^C(\lfloor nx\rfloor) = \lim_{n\to\infty}\sum_{j=0}^{\lfloor nx\rfloor}\left\{\sum_{\ell=0}^{n}|v_\ell(j)|^2|v_\ell(0)|^2\right\} = \bar{F}(x), \quad (2)$$

where $\lfloor a\rfloor$ denotes the biggest integer which is not greater than a.

From Eq. (2) and the relation

$$\begin{aligned}
\mathbb{P}\left(\frac{\bar{X}_n^D}{n} \le x\right) &= \bar{F}_n^D(nx) = \bar{F}_n^D(\lfloor nx\rfloor)\\
&= \bar{F}_n^C(\lfloor nx\rfloor)\\
&+ \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}\left\{-p_{\lfloor nx\rfloor}^R|v_\ell(\lfloor nx\rfloor)|^2 + p_{\lfloor nx\rfloor+1}^L|v_\ell(\lfloor nx\rfloor+1)|^2\right\}|v_\ell(0)|^2,
\end{aligned}$$

if we can prove

$$\lim_{n\to\infty}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}|v_\ell(\lfloor nx\rfloor)|^2|v_\ell(0)|^2 = \lim_{n\to\infty}\sum_{\ell=1}^{n-1}\frac{1}{1-\lambda_\ell^2}|v_\ell(\lfloor nx\rfloor+1)|^2|v_\ell(0)|^2 = 0, \quad (3)$$

then we can conclude

$$\lim_{n\to\infty}\mathbb{P}\left(\frac{\bar{X}_n^D}{n} \le x\right) = \bar{F}(x),$$

for all points at which $\bar{F}$ is continuous.

Now we show an example for the convergence. That is $\limsup_{n\to\infty}\lambda_1 < 1$ case. By the definition, we obtain

$$0 \le \sum_{j=0}^{\lfloor nx\rfloor}\left\{\sum_{\ell=1}^{n-1}|v_\ell(j)|^2|v_\ell(0)|^2\right\} \le \bar{F}_n^C(\lfloor nx\rfloor) \xrightarrow{n\to\infty} \bar{F}(x).$$

Also we have

$$0 \le \sum_{j=0}^{\lfloor nx\rfloor+1}\left\{\sum_{\ell=1}^{n-1}|v_\ell(j)|^2|v_\ell(0)|^2\right\} \le \bar{F}_n^C\left(\left\lfloor n\left(x+\frac{1}{n}\right)\right\rfloor\right) \xrightarrow{n\to\infty} \bar{F}(x),$$

from continuity of $\bar{F}$ at x. These mean that

$$\lim_{n\to\infty}\sum_{\ell=1}^{n-1}|v_\ell(\lfloor nx\rfloor)|^2|v_\ell(0)|^2 = \lim_{n\to\infty}\sum_{\ell=1}^{n-1}|v_\ell(\lfloor nx\rfloor+1)|^2|v_\ell(0)|^2 = 0. \quad (4)$$

Therefore combining with Eq. (4), we obtain Eq. (3) as follows:

$$\limsup_{n\to\infty} \sum_{\ell=1}^{n-1} \frac{1}{1-\lambda_\ell^2} |v_\ell(\lfloor nx \rfloor)|^2 |v_\ell(0)|^2$$
$$\leq \limsup_{n\to\infty} \frac{1}{1-\lambda_1^2} \sum_{\ell=1}^{n-1} |v_\ell(\lfloor nx \rfloor)|^2 |v_\ell(0)|^2$$
$$\leq \frac{1}{1-\limsup_{n\to\infty} \lambda_1^2} \times \lim_{n\to\infty} \sum_{\ell=1}^{n-1} |v_\ell(\lfloor nx \rfloor)|^2 |v_\ell(0)|^2$$
$$= 0,$$
$$\limsup_{n\to\infty} \sum_{\ell=1}^{n-1} \frac{1}{1-\lambda_\ell^2} |v_\ell(\lfloor nx \rfloor + 1)|^2 |v_\ell(0)|^2$$
$$\leq \limsup_{n\to\infty} \frac{1}{1-\lambda_1^2} \sum_{\ell=1}^{n-1} |v_\ell(\lfloor nx \rfloor + 1)|^2 |v_\ell(0)|^2$$
$$\leq \frac{1}{1-\limsup_{n\to\infty} \lambda_1^2} \times \lim_{n\to\infty} \sum_{\ell=1}^{n-1} |v_\ell(\lfloor nx \rfloor + 1)|^2 |v_\ell(0)|^2$$
$$= 0.$$

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