# L2 8/02: Discrete walks

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# Perfect State Transfer

Let $z$ be a unit vector in $\mathbb{C}^d$. Define a density

$$D_{u,z} := e_u e_u^T \otimes z z^*$$

$$(e_u \otimes z)(e_u \otimes z)^T$$

**Lemma** If $U^k D_{u,\mathbb{1}} U^{-k} = D_{u,z}$ and $\|z\|=1$

then $z = \frac{1}{\sqrt{d}} \mathbb{1}$.

**Proof** Assume $A$ has spectral decomposition $A = \sum_r \lambda_r F_r$

Then $U = \sum_r e^{i\lambda_r} F_r$ and

$$U^k D_{\underset{\sim}{u},\underset{\sim}{1}} U^{-k} = D_{v,\underset{\sim}{z}}$$

Since $U$ & $D_{\underset{\sim}{u},\underset{\sim}{1}}$ are real, $D_{v,\underset{\sim}{z}}$ is real and so $\underset{\sim}{z}$ is real.

As $U(\underset{\sim}{1}\otimes\underset{\sim}{1}) = \underset{\sim}{1}\otimes\underset{\sim}{1}$, we have:

$$(\underset{\sim}{1}\otimes\underset{\sim}{1})^T D_{v,\underset{\sim}{z}} (\underset{\sim}{1}\otimes\underset{\sim}{1}) = (\underset{\sim}{1}\otimes\underset{\sim}{1})^T (e_n e_n^T \otimes \underset{\sim}{z}\underset{\sim}{z}^*)(\underset{\sim}{1}\otimes\underset{\sim}{1}) = \underset{\sim}{1}^T \underset{\sim}{z}\underset{\sim}{z}^* \underset{\sim}{1}$$

$$(\underset{\sim}{1}\otimes\underset{\sim}{1})^T D_{\underset{\sim}{u},\underset{\sim}{1}} (\underset{\sim}{1}\otimes\underset{\sim}{1}) = \frac{1}{d} \underset{\sim}{1}^T\underset{\sim}{1}\, \underset{\sim}{1}^T\underset{\sim}{1} = d$$

and therefore $\langle \underset{\sim}{1}, \underset{\sim}{z} \rangle = \sqrt{d}$. By Cauchy-Schwarz.

$$\langle \underset{\sim}{1}, \underset{\sim}{z} \rangle^2 \leq \langle \underset{\sim}{1}, \underset{\sim}{1} \rangle \langle \underset{\sim}{z}, \underset{\sim}{z} \rangle = d$$

Equality holds if & only if $\underline{z} = c\underline{1}$, when $\underline{z} = \underline{1}$. $\square$

If $U^k D_{u,\underline{z}} U^{-k} = D_{v,\underline{1}}$, we say we have

==perfect state transfer== from $u$ to $v$.

==Exercise== $U^k D_{u,y} U^{-k} = D_{v,\underline{z}}$, $\|y\| = \|\underline{z}\| = 1$, $y$ real $\Rightarrow \underline{z} = y$

Recall that, for continuous walks, if

$$D_2 = U(t) D_1 U(-t)$$

and $D_1, D_2$ are real, then taking complex conjugates yields

$$D_2 = \bar{D}_2 = U(-t) \bar{D}_1 U(t) = U(-t) D_1 U(t)$$

and therefore $D_1 = U(t) D_2 U(-t)$

What about discrete walks?

Assume

$$D_2 = U^k D_1 U^{-k}$$

with $D_1, D_2$ real. Then

$$D_2 = \bar{D}_2 = \bar{U}^k D_1 \bar{U}^{-k}$$

and then $D_1 = \bar{U}^{-k} D_2 \bar{U}^k$.

Since $\bar{U}^{-1} \neq U$ (in general), this gives us nothing.

But still:

**Theorem** (H. Zhan) Let $U$ be the transition matrix for the arc-reversal walk on $X$ and assume $u, v \in V(X)$.

If $U^k D_{u,\underline{1}} U^{-k} = D_{v,\underline{1}}$, then $U^k D_{v,\underline{1}} U^{-k} = D_{u,\underline{1}}$. $\square$

This result is a consequence of the following characterization of perfect state transfer.

(H. Zhan)

**Theorem** The arc-reversal walk on $X$ (k-regular) has perfect state transfer from $u$ to $v$ at time $k$ if & only if all of the following hold:

(a) For each $\lambda$, we have $E_\lambda e_u = \pm E_\lambda e_v$.

(b) If $E_\lambda e_u = E_\lambda e_v \neq 0$, there is an even integer $j$ s.t. $\lambda = d\cos(j\pi/k)$

(c) If $E_\lambda e_u = -E_\lambda e_v \neq 0$, there is an odd integer $j$ s.t. $\lambda = d\cos(j\pi/k)$. $\square$

Since these conditions are symmetric in $u$ & $v$, the theorem follows.

Question Does this theorem hold for 2-reflection walks based on biregular bipartite graphs?

Mixing

$U$ unitary $\Rightarrow$ $U = \exp(iH)$ $H$ Hermitian

Hamiltonian

$$U^k = \exp(k\,iH)$$

Much of the theory of continuous quantum walks carries over to discrete walks. We consider one case of this: mixing.

If the initial state of a discrete walk is $D_0$, the state at time $k$ is

$$D_k := U^k D_0 U^{-k}$$

We define the average state to be

$$\lim_{K\to\infty} \frac{1}{K} \sum_{m=0}^{K-1} U^m D_0 U^{-m}$$

and denote it by $\hat{D}_0$. If $U = \sum_r e^{i\theta_r} F_r$ is the spectral decomposition of $U$, we have

$$U^m D_0 U^{-m} = \sum_{r,s} e^{im(\theta_r - \theta_s)} F_r D_0 F_s$$

$$= \sum_r F_r D_0 F_r + \sum_{r \neq s} e^{im(\theta_r - \theta_s)} F_r D_0 F_s$$

We see that

$$\frac{1}{K}\sum_{m=0}^{K-1} e^{im(\theta_r-\theta_s)} = \frac{1}{K}\,\frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}$$

and accordingly

$$\frac{1}{K}\sum_{m=0}^{K-1} U^k D_0 U^{-k} = \sum_r f_r D_0 f_r + \frac{1}{K}\left(\sum_{r\neq s} \frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}\right) f_r D_0 f_s$$

If $r\neq s$, then for any $K$

$$\left|\frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}\right| \leq \frac{2}{\left|1-e^{i(\theta_r-\theta_s)}\right|}$$

So we have:

**Theorem** If $U$ is unitary with spectral decomposition $U = \sum_r e^{i\theta_r} F_r$, the average state of the discrete walk based on $U$ & starting at $D_0$ is $\sum_r F_r D_0 F_r$. $\square$

Since $U(F_r D_0 F_r)U^{-1} = \theta F_r D_0 F_r \theta^{-1} = F_r D_0 F_r$, it follows that the average state $\hat{D}_0$ commutes with $U$.

Assume $\alpha \in \text{arcs}(X)$. The probability that, after $k$ steps starting from $D_\alpha$, the walker is on $\alpha$ is

$$\langle D_k, e_\alpha e_\alpha^T \rangle = e_\alpha^T D_k e_\alpha = (D_k)_{\alpha,\alpha}$$

If $\beta$ is an arc and $D_0 = e_\beta e_\beta^T$ then

$$\langle D_k, e_\alpha e_\alpha^T \rangle = \langle U^k e_\beta e_\beta^T U^{-k}, e_\alpha e_\alpha^T \rangle$$

$$= \operatorname{tr}(e_\alpha e_\alpha^T U^k e_\beta e_\beta^T U^{-k})$$

$$= (U^k)_{\alpha,\beta} (U^{-k})_{\beta,\alpha}$$

Applying the spectral decomposition, we rewrite this as

$$\sum_r e^{ik\theta_r}(F_r)_{\alpha,\beta} \sum_s e^{-ik\theta_s}(F_s)_{\beta,\alpha}$$

$$= \sum_{r,s} e^{ik(\theta_r-\theta_s)}(F_r)_{\alpha,\beta}(F_s)_{\beta,\alpha}$$

So:

$F_s^T = \bar{F}_s$

**Lemma** For a discrete walk starting on the arc $\alpha$, the average probability that the walker is on the arc $\beta$ is $\sum_r (F_r \circ \bar{F}_r)_{\alpha\beta}$.

We define the average mixing matrix of a discrete walk to be

$$\hat{M} = \sum_r F_r \circ \bar{F}_r$$

You may show that

$$\hat{M} = \lim_{K\to\infty} \frac{1}{K} \sum_{m=0}^{K-1} U^m \circ \bar{U}^m .$$

**Lemma** The average mixing matrix $\hat{M}$ is positive semidefinite. All eigenvalues of $\hat{M}$ lie in $[0,1]$.

**Proof.** If $F$ is Hermitian, so is $\bar{F}$, and $F$ & $\bar{F}$ have the same eigenvalues. So if $U = \sum_r e^{i\theta_r} F_r$, then $F_r \succeq 0$ and $\bar{F}_r \succeq 0$. By Schur's theorem this implies that $F_r \circ \bar{F}_r \succeq 0$ and so $\hat{M} = \sum_r F_r \circ \bar{F}_r \succeq 0$.

For the second claim,

$$I = I \circ I = \left(\sum_r F_r\right) \circ \left(\sum_s \bar{F}_s\right) = \hat{M} + \sum_{r \neq s} F_r \circ \bar{F}_s$$

Therefore $I - \hat{M} \geq 0$. $\square$

Uniform average mixing

A quantum walk has uniform average mixing if $\hat{M}$ is flat. We aim to characterize when this can happen.

**Lemma** If $\overset{n\times n}{U} = \sum_r e^{i\theta_r} F_r$ and $\mu_r$ is the multiplicity of $\theta_r$, then $\mathrm{tr}(\hat{M}) \geq \frac{1}{n} \sum_r \mu_r^2$. Equality holds if & only if each idempotent has constant diagonal.

**Proof** We have $\mu_r = \mathrm{tr}(F_r)$ and, applying Cauchy-Schwarz

$$\frac{1}{n}\sum_r \mu_r^2 = \frac{1}{n}\sum_r \mathrm{tr}(F_r)^2 \leq \mathrm{tr}(F_r \circ F_r)$$

and so $\mathrm{tr}(A) \geq \frac{1}{n}\sum_r \mu_r^2$. Equality holds if & only if $F_r$ has constant diagonal, for each $r$. $\square$

**Corollary** We have $\operatorname{tr}(\hat{M}) \geq 1$ and equality holds if & only if $\mu_r = 1$ and $F_r$ is flat, for all $r$.

**Proof** We have $\sum_r \mu_r = n$ and

$$0 \leq \sum_r \left(\mu_r - \frac{\sum \mu_r}{n}\right)^2 = \sum_r (\mu_r - 1)^2 = \sum_r \mu_r^2 - n$$

Hence $\frac{1}{n} \sum \mu_r^2 \geq 1$. If equality holds $\mu_r = 1$ $\forall r$. Now $F_r$ is a rank-1 matrix with constant diagonal, so it is flat. $\square$

skew adj. matrix $S$, $Q \pm I$, $S^T = -S$

$\exp(tS)$ is orthogonal

**Theorem** For a discrete walk, the following are equivalent:

(a) The walk has uniform average mixing.

(b) $tr(\widehat{M}) = 1$

(c) The eigenvalues of $U$ are simple and its spectral projections are flat.

**Proof** If we have uniform average mixing, $\hat{M} = \frac{1}{n} J$

and $tr(\hat{M}) = 1$, so (a) $\Rightarrow$ (b).

From the corollary, (b) $\Rightarrow$ (c). If (c) holds,

$$\hat{M} = \sum_r F_r \circ \bar{F}_r$$

and $F_r \circ \bar{F}_r$ is flat. $\square$

# L28/01, part II

# Shunts

Other walks

We have been focused on arc-reversal walks. We briefly discuss some of the alternatives.

Our approach to spectral decomposition works well for the 2-reflection walks coming from bipartite graphs, in particular biregular bipartite graphs. It can also handle arc-reversal walks on non-regular graphs (replace $A$ by the normalized Laplacian).

We discuss shunt-decomposition walks, which are not 2-reflection walks. A shunt decomposition of a $d$-regular digraph is a set of permutation matrices $P_1, \ldots, P_d$ such that $A = P_1 + \cdots + P_d$. Given such a shunt decomposition, we define

$$S = \begin{bmatrix} P_1^{-1} & & \\ & \ddots & \\ & & P_d^{-1} \end{bmatrix}$$

So $S$ is a permutation matrix of order $nd \times nd$.

Let $C$ be a $d \times d$ unitary matrix (a coin). The matrix

$$U = S(C \otimes I_n)$$

is unitary, and so it the transition matrix of a shunt decomposition walk.

In general, neither $S$ nor $C \otimes I_n$ have order two.

We can make some progress, but first:

**Lemma** If $X$ is a $d$-regular digraph, it admits a shunt decomposition.

Proof. Let $B$ be the adjacency matrix of $X$ and set

$$A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}.$$

Then $A$ is the adjacency matrix of a $d$-regular bipartite graph, $Y$ say, and $Y$ admits a 1-factorization

Equivalently there are permutation matrices $Q_1, \ldots, Q_d$ such that $Q_r^2 = I$ & $\sum_r^d Q_r = A$. We have

$$Q_r = \begin{pmatrix} 0 & P_r \\ P_r & 0 \end{pmatrix}$$

for a permutation matrix $P_r$, and $P_1, \ldots, P_d$ is a shant decomposition of $X$. $\square$

**Remark:** if $X$ is the complete digraph on $n$ vertices, with a loop on each vertex ($A(X) = J$), then shunt decompositions of $X$ correspond to $n \times n$ Latin squares