Szegedy walks Dan D 29/06/2018

SZEGEDY QUANTUM WALKS DEMYSTIFIED

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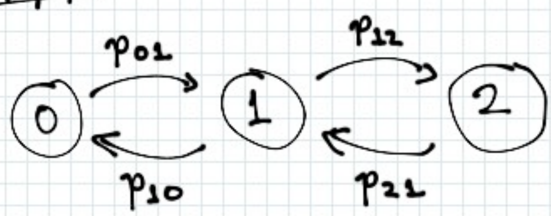
Paper Mario Szegedy, FOCS 2004

Outline

- Classical Markov chains, hitting + quantisation
- Szegedy's construction
- Spectrum of the walk matrix
- Hitting time of the quantum walk

Markov chain given by transition matrix P indexed by state space X.

Example



$$P = \begin{pmatrix} 0 & p_{01} & 0 \\ p_{10} & 0 & p_{12} \\ 0 & p_{21} & 0 \end{pmatrix}$$

$$X = \{0, 1, 2\}$$

Move from state x to y with probability $p_{x,y}$

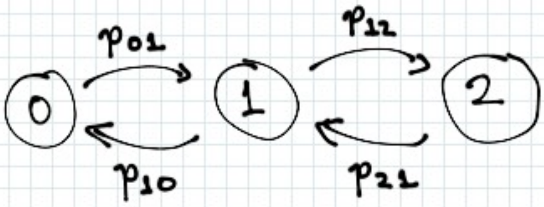
Dynamics: Start with distribution x_0 over X. Then, state at time t is $x_t = x_0 P^t$ (Note: x_t is a row vector, multiply P from right)

Def^n Stationary distribution π is the distribution (unique for ergodic Markov chain) satisfying $\pi = \pi P$.

Task find a marked element $M \subseteq X$. Hitting time is expected # of timesteps to reach an element of M from given starting distribution.

Classically, hitting time is given by $O\left(\frac{1}{1-\lambda_2}\right)$, where $1 = \lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_{|X|}$ are the eigenvalues of P. We call $1-\lambda_2$ the spectral gap.

QUANTISING A CLASSICAL WALK

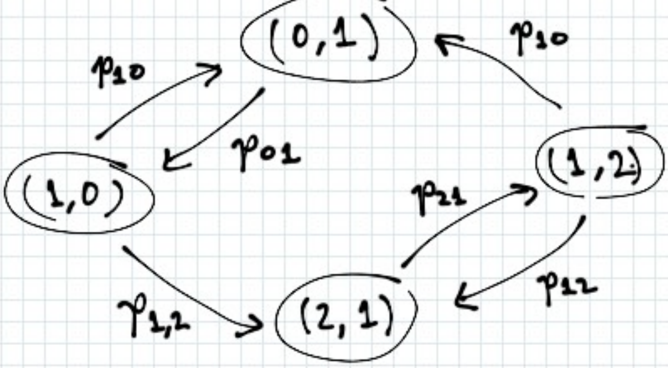


Why?. to make correspondence btwn classical + quantum clear. It's not possible to quantise a walk on vertices (Simone!, 2005)

Let's envision a walk on the arcs

arc $(u,v) \to (x,y)$
iff $u = y$

Note if condition was $v = x$ then this is line graph of X.



<u>Interpretation:</u> $(x,y) \equiv$ "state of walk P is currently x, it was y at previous step"

State space is now $X \times X$

What about dynamics?

Split transition into "flip", then "shift"

$$\delta_{u,y} = \begin{cases} 1, & u=y; \\ 0, & \text{o/w}. \end{cases}$$

Define 'left' coin flip matrix F^L where

$$F^L_{(u,v),(x,y)} = \delta_{v,y} \cdot p_{y,x} \quad \text{mixes left}$$

also, "right" flip matrix F^R:

$$F^R_{(u,v),(x,y)} = \delta_{u,x} \cdot p_{x,y} \quad \text{mixes right}$$

Define shift matrix S such that $S: e_{(x,y)} \mapsto e_{(y,x)}$

One walk step is $S \cdot F^L$ (this is a transition matrix)

since $(SF^L)_{(u,v),(x,y)} = \delta_{u,y}\, p_{y,x}$ $[(y,v) \mapsto (x,y)$ with prob. $p_{y,x}$ for any $v \in X]$

Aside: the Markov chain SF^L with the homomorphism $(x,y) \mapsto x$ is a "lifted" Markov chain of P.

How to quantise?

Coined walks: Relax F^L to a unitary coin $\quad C_{(u,v),(x,y)} = 0$ when $v \neq y,\ x \neq y$

Szegedy does something different.

FACT $SF^L SF^L = F^R F^L$

$\Rightarrow$ one application of $F^R F^L$ is equivalent to two random walk steps.

We are going to "quantise" F^L & F^R

Our Hilbert space $\mathcal{H} = \text{span}\{|x\rangle|y\rangle \mid x, y \in X\}$

Define $\phi_x = \sum_{y \in X} \sqrt{p_{x,y}}\, |x\rangle|y\rangle$, $\psi_y = \sum_{x \in X} \sqrt{p_{y,x}}\, |x\rangle|y\rangle$

& matrices

$A = (\phi_1 \;\; \phi_2 \cdots \phi_{|X|})$, $B = (\psi_1 \;\; \psi_2 \; \cdots \; \psi_{|X|})$

$A, B \in \mathbb{R}^{|X|^2 \times |X|}$

Define $R_R = 2\underbrace{A \cdot A^*}_{\Pi_{col(A)}} - I$, $R_L = 2\underbrace{B \cdot B^*}_{\Pi_{col(B)}} - I$

R_R & R_L are reflections about subspaces spanned by A & B respectively.

$$\boxed{\text{Walk operator } W_p = R_R R_L}$$

R_R, R_L are real, orthogonal operators on $\mathcal{H}$

How is W_P a quantisation of the classical walk?

$F^R \mapsto R_1$, $F^L \mapsto R_2$

F^L mixes left endpoints of edges with neighbours.

F^R mixes right endpoints of edges with neighbours.

If the $p_{x,y}$ are equal for all $y : (x,y) \in E(G)$ then R_1, R_2 are Grover diffusion operators.

Spectrum of W

Thm (classical result (Horn & Johnson Cor 2.5.11))

Let $A \in \mathbb{R}^{n \times n}$. $A \cdot A^T = I$ iff $\exists$ real/orthogonal $Q \in \mathbb{R}^{n \times n}$ & $p \in \mathbb{Z}_{\geq 0}$ such that $Q^T A Q$ takes the form

$$\underbrace{I_r}_{\text{identity}} \oplus \underbrace{(-I_s)}_{\text{reflection about the origin}} \oplus \underbrace{\begin{bmatrix} \cos\theta_1 & \sin\theta_1 \\ -\sin\theta_1 & \cos\theta_1 \end{bmatrix}}_{\text{rotation in 2D subspace}} \oplus \cdots \oplus \begin{bmatrix} \cos\theta_p & \sin\theta_p \\ -\sin\theta_p & \cos\theta_p \end{bmatrix},$$

where $r+s+2p=n$ & each $\theta_j \in (0, 2\pi)$. Eigenvalues are $1, -1$ & $e^{\pm i\theta_1}, \dots, e^{\pm i\theta_p}$.

$Q \cdot - Q^T \equiv$ "there is an orthonormal basis in which A takes desired form"

Def^n Discriminant matrix

$$D(A,B) = A^* B.$$

$D(A,B)$ is spectrally similar to P

Note: $[D(A,B)]_{x,y} = \sqrt{p_{x,y} \cdot p_{y,x}}$

We can view $v \mapsto D(A,B)v$ as a map from $col(B) \to col(A)$ considering v expressed in eigenbasis of B

Likewise $D^*(A,B)$ map from $col(A) \to col(B)$.

What Szegedy does is relates the singular value decomposition of $D(A,B)$ to the eigendecomposition of W.

Let w_k, v_k be a left-right singular value pair of unit vectors for $D(A,B)$, with singular value σ_k.

Then, $D(A,B)v_k = \sigma_k w_k$

$$D(A,B)^* w_k = \sigma_k v_k$$

Recall, $A^T A = B^T B = I_{|X|}$

Lem. singular values of $D(A,B)$ in $(0,1) \cup \{1,-1\}$

Can associate angle $\sigma_k = \cos\theta_k$ between Aw_k, Bv_k

$$w_k^\dagger A^\dagger B v_k = \cos\theta_k \quad , \quad \theta_k \in (0, \tfrac{\pi}{2}]$$

Can check:

$$R_1 R_1^T = R_2 R_2^T = I$$

$\Rightarrow R_1 R_2$ is real orthogonal matrix

$\Rightarrow$ decomposes into direct sum of identity, negative identity and rotations in two-dimensional subspaces

Szegedy shows that these two-dimensional subspaces are span$\{Aw_k, Bv_k\}$ with eigenvalues $e^{\pm 2i\theta_k}$, eigenvectors $Aw_k - e^{\pm i\theta_k} Bv_k$ (unnormalised)

(corresponding to singular values $\sigma_k \in (0,1)$) $\quad col(A) \cup col(B)$

W acts as identity on $col(A) \cap col(B)$, $col(A)^\perp \cap col(B)^\perp$

$\sigma_k = +1$

W acts as reflection about origin on $col(A)^\perp \cap col(B)$,

$col(A) \cap col(B)^\perp$

$\sigma_k = -1$

So we have full control of the spectrum of W!

Hitting times

First we define a modified walk with matrix

$$P' = \begin{pmatrix} P_{X\setminus M} & P'' \\ 0 & I_M \end{pmatrix}$$

P_Q is the submatrix of P on index set $Q \subseteq [n]$

Once walk reaches a marked vertex, stays there!

<u>Corollary</u> If our walk P has stationary distribution π,

$$\| \pi (P')^t - \pi \|_1 = \pi (P')^t \underline{1}_M - \pi_M \underline{1}_M$$

probability of being at marked vertex time t

$\underline{1}_M$: all-ones vector on set M, zero otherwise

$\| \pi (P')^t - \pi \|_1$ large when M is likely to have been hit i.e. $\pi (P')^t \underline{1}_M$ is large

<u>Def^n</u> (Quantum hitting time)

Number of steps, T_0, for which

$$\frac{1}{T+1} \sum_{t=0}^{T} \| W_{P'}^t \phi_0 - \phi_0 \|_2 \geq 1 - \frac{|M|}{|X|} \quad \text{for all } T \geq T_0,$$

appropriately chosen initial state ϕ_0

Remarks

i. Using ℓ_2 as opposed to ℓ_1-norm

ii. Time-averaged, this is because unitary dynamics prevents convergence of $W_{P'}^t \phi_0$

iii. Condition $\|W_{P'}^t \phi_0 - \phi_0\|_2 \geq 1 - \frac{|M|}{|X|} \not\Rightarrow$ measuring $W_{P'}^t \phi_0$ gives marked element with constant probability. With more work, Szegedy turns this into a search algorithm

Comparison with classical hitting time

Classically, have $O\left(\frac{1}{1-\lambda_2}\right)$ hitting time

Call $1-\lambda_2 =: \delta$. (spectral gap)

Szegedy shows that $T_0 = O\left(\frac{1}{\sqrt{1-\lambda_2}}\right)$ (ergodic, reversible chain P)

Proof decomposes ϕ_0 into subspaces of $W_{P'}$, most important eigenvalue is λ_2.

Very rough explanation

Defn Phase gap $\Delta := 2\theta$, where θ smallest angle in $\left(0, \frac{\pi}{2}\right]$ such that $\cos\theta$ is a singular value of $D(A,B)$

Angular distance of 1 from any other eigenvalue of W on $\mathrm{col}(A) \cup \mathrm{col}(B)$ is at least Δ.

For an ergodic, reversible P, $\delta = 1 - \cos\theta$, $\Delta = 2\theta$.

$$\Delta = 2\theta \geq |1 - e^{2i\theta}| \; 2\sqrt{1-\cos^2\theta} \geq 2\sqrt{\delta}.$$

This is the origin of quadratic speedup in hitting time!

Phase gap most prominent term in proof.