Markov chains quantum walk qubitization

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2/12

$\Sigma \cong [n]$ state space   probability dist $\mathbb{P}: \Sigma \to [0,1]$

$i \in \Sigma$ $\mathbb{P}(i) = P_i \geq 0$ $\sum_{i \in \Sigma} \mathbb{P}(i) = 1$

$p, q \in \mathbb{R}^N$ $q = P p$ P is transition matrix $(\mathbb{R}^{N \times N})$

map a prob dist $\to$ prob dist

$$\begin{cases} P_{ij} \geq 0 \\ \sum_i P_{ij} = 1 \end{cases} \qquad q_i = \sum_j P_{ij} p_j$$

$$1 = \sum_i q_i = \sum_j \left(\sum_i P_{ij} \right) p_j = \sum_j p_j$$

column stochastic
(left stochastic)

Markov chain on Σ: a sequence of random variables $X_1, \dots, X_t, \dots \in \Sigma$

Markov property: $\mathbb{P}(X_{t+1} = i \mid X_t = j, X_{t-1} = j_{t-1}, \dots, X_1 = j_1) = \underbrace{\mathbb{P}(X_{t+1} = i \mid X_t = j) = P_{ij}}_{\text{time homogeneous}}$

stationary distribution. $\pi \in \mathbb{R}^N$ $\sum_i \pi_i = 1$

$P\pi = \pi$

Goal: prepare π (classically)

$|\pi\rangle := \sum_i \sqrt{\pi_i}\, |i\rangle$ (quantumly) coherent representation of π

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observable O $\mathbb{E}_\pi O = \sum_i O_i \pi_i \approx \frac{1}{N_s} \sum_{j=1}^{N_s} O_{x_j}$ $x_j \sim \pi$

$$\hat{O} = \sum_i O_i |i\rangle\langle i| \qquad \langle \pi | \hat{O} | \pi \rangle = \mathrm{Tr}[\underbrace{|\pi\rangle\langle\pi|}_{\rho} O]$$

Ex. $\Sigma = \{0,1\}^n \cong \{0, 1, \dots, N-1\}$ $N = 2^n$

j   11001010
i   10001010

$$P_{ij} = \begin{cases} \frac{1}{n} & \text{if } i, j \text{ differ by a bit} \\ 0 & \text{otherwise} \end{cases}$$

$\pi_i = \frac{1}{N}$ $\sum_j P_{ij} \pi_j = \frac{1}{N} \sum^{n} \frac{1}{n} = \frac{1}{N} = \pi$

start from arbitrary ρ

$$\|P^t_\rho - \pi\|_1 \xrightarrow{t\to\infty} 0 \qquad \le C(1-\gamma)^t$$

total variation — spectral gap

$$\|q-q'\|_1 = \sum_i |p_i - q_i|$$

$t \sim \frac{1}{\gamma}\log 1/\epsilon$

quantumly $t \sim \frac{1}{\sqrt{\gamma}}$

Szegedy 04'

reversibility: if $\forall i,j$ $P_{ij}\pi_j = P_{ji}\pi_i$

detailed balance

$\boxed{\text{f.a.i.r.}}$ MCs

$E(i)$ energy

prepare Gibbs distribution $\pi_i = \frac{1}{Z} e^{-\beta E(i)}$ $\quad Z = \sum_i e^{-\beta E(i)}$ partition func

$\beta = 0 \quad \pi_i = \frac{1}{N}$ infinite temp $(1/\beta)$

(in example) replace P_{ij} with Q_{ij}

$Q_{ij} = Q_{ji}$ proposal

Metropolis-Hastings accept/reject step $\alpha_{ij} = \min\{1, e^{-\beta(E(i)-E(j))}\}$

$$P_{ij} = \begin{cases} Q_{ij}\alpha_{ij} & \text{if } i,j \text{ differ by a bit} \to \text{accept} \\ 1-\Sigma & \text{if } i=j \\ 0 & \text{otherwise} \end{cases}$$

<u>Claim</u>: $\sum_j P_{ij}\pi_j = \pi_i$

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bad scenario 1: π_1 not unique π

π_2 $\quad \alpha\pi_1 + (1-\alpha)\pi_2 \quad \forall \alpha\in[0,1]$

fix: irreducible: $\forall i,j \in \Sigma$, exist $t>0$ s.t. $(P^t)_{ij} > 0$

bad scenario 2:

$1-p \quad p$

"stationary dist won't be unique"
"even + odd", "period"

$$\mathcal{T}(i) = \{t \ge 1 : P^t(i,i) > 0\}$$

period at $i := \gcd(\mathcal{T}(i))$

$\pi_{1,2,3,4}$

aperiodic period of every state $i = 1$

$p = \frac{1}{2} \quad \pi_i = \frac{1}{4} \quad \pi = \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \\ 0 \end{pmatrix} \quad P^2 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}, \quad \pi^{(1)} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix} \quad \pi^{(2)} = \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}$

$P^2\pi^{(1)} = \pi^{(1)}$
$P^2\pi^{(2)} = \pi^{(2)}$

Fact: finite irreducible aperiodic MC.

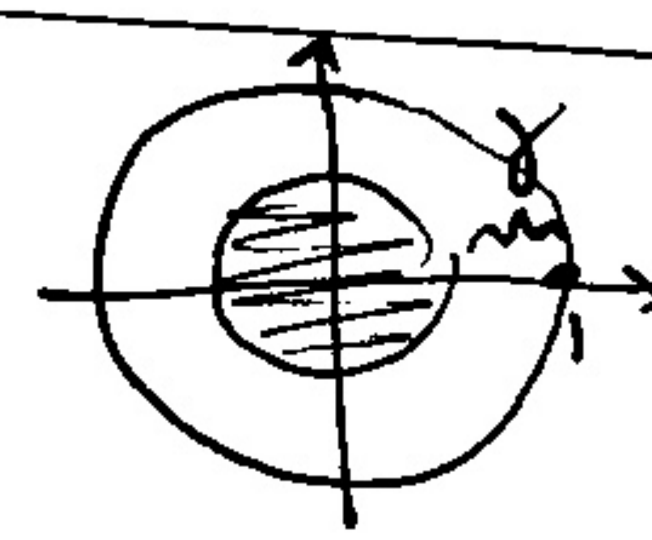
$\exists\, t \ge 1$ s.t. $P^t(i,j) > 0$, $\forall i,j$

$P = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & & \\ 0 & & & \end{pmatrix}$ $\quad P^t = \begin{pmatrix} >0 & >0 \end{pmatrix}$ positive matrix (not positive semidefinite; different concept)

Thm (Perron) A positive, there exists a simple eigenvalue $\lambda = \rho(A)$ ("spectral radius") where $\rho(A) = \max_i \{|\lambda_i|\}$. $Av = \lambda v$, unique eigenvector v can be chosen to have $v_i > 0, \forall i$; all other eigenvalues $|\lambda'| < \rho(A)$

"simple", $\begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}$ $\begin{pmatrix} \lambda & 1 \\ & \lambda \end{pmatrix}$ not simple; must look like $\left(\begin{array}{c|c} \lambda & 0 \\ \hline 0 & \end{array}\right)$

~~prop.~~ finite irreducible aperiodic MC with transition P, then unique stationary dist π, exist ~~$\gamma\dots$~~ $\gamma \in (0,1]$ all other eigenvalues $|\lambda| \le 1-\gamma$



pf. (1) $P^t\pi = \pi$ $\quad (\rho(P^t) = 1)$

$P^t(P\pi) = P\pi$, by uniqueness $P\pi = \pi$

(2) $Pv = \lambda v$, $\lambda \ne 1$. $P^t v = \lambda^t v$. we know $|\lambda^t| \le 1-\gamma'$, ~~...~~ $\gamma' \in (0,1]$

$\rightarrow |\lambda| \le (1-\gamma')^{1/t} =: 1-\gamma$

$\pi_j = \frac{1}{Z} e^{-\beta E(j)}$

$P_{ij}\pi_j = \frac{1}{n}\min\{1, e^{-\beta(E(i)-E(j))}\} \cdot e^{-\beta E(j)}$

i,j differ by a bit

if $E(i) \le E(j)$ $\quad P_{ij}\pi_j = \frac{1}{Zn} e^{-\beta E(j)} = P_{ji}\pi_i = \frac{1}{Zn} \cdot \left(e^{-\beta(E(j)-E(i))}\right) \cdot e^{-\beta E(i)}$

detailed balance $\boxed{P\pi = \pi}$

f.a.i.r. Define discriminant $D_{ij}=\sqrt{P_{ij}P_{ji}}$, real / symmetric

<u>Lem</u> $D=\mathrm{diag}(\pi^{-\frac{1}{2}})\,P\,\mathrm{diag}(\pi^{1/2})$