Markov chains: memory 1 $\qquad W_{ij}$ stochastic matrix

update rule $\quad p_j(t+1) = \sum_i W_{ji}\, p_i(t)$

$$\vec{p}(t+1) = W\, \vec{p}(t)$$

$W \cdot \vec{w}^{(1)} = \vec{w}^{(1)} \;\to\; \vec{w}^{(1)}$ = stationary distribution

Th 1: MC irreducible + pos. recurrent $\left(\langle T_i \rangle < +\infty\right)$

$\Rightarrow \vec{w}^{(1)}$ <u>unique</u> stat. distr. $\to w_i^{(1)} = \dfrac{1}{\langle T_i \rangle}$

Th 2: MC irreducible + pos. recurr.

+ aperiodic ($\to$ period 1)

CONVERGENCE $\quad p_j(t) = \sum_i (W^t)_{ji}\, p_i(0) \xrightarrow[t \to \infty]{} w_j^{(1)}$

(Perron-Frobenius theorem) $\quad \lambda^{(1)} = 1 > |\lambda^{(2)}| \geq |\lambda^{(3)}| \dots$

(ERGODIC MC)

$\vec{p}(t) = \sum_k \alpha_k \vec{w}^{(k)} \to$ right eigenvectors

$\alpha_k(t) = \vec{p}(t) \cdot \vec{w}_\ell^{(k)} \to$ left eigenvectors

$$\vec{p}(t) = W^t \vec{p}(0) = W^t \left[\sum_k \alpha_k(0)\, \vec{w}^{(k)}\right]$$

$$= \sum_k \alpha_k(0) \left(\lambda^{(k)}\right)^t \vec{w}(k)$$

$$\alpha_k(t) = \alpha_k(0) \left[\lambda^{(k)}\right]^t$$

$$\lambda^{(k)} = |\lambda^{(k)}| \cdot \exp(i \phi_k)$$

$$\alpha_k(t) = \alpha_k(0)\, \exp(i t \phi_k)\, |\lambda^{(k)}|^t$$

$$= \alpha_k(0)\, \exp(i t \phi_k)\, \exp(-t/\tau_k)$$

$$\tau_k = -1/\ln(|\lambda_k|) > 0 \qquad |\lambda_k| < 1$$
$$(k \geq 2)$$

$$\to \vec{p}(t) = \alpha_1(0)\, \vec{w}^{(1)} + \underbrace{\alpha_2(0)\exp(it\phi_2)\exp(-t/\tau_2)}_{\text{leading term}} + \dots$$

$$|\lambda^{(2)}| > |\lambda^{(k)}| \quad (k > 2) \quad \tau_2 > \tau_k$$

characteristic time for convergence to stationarity

$$\to \underbrace{\tau_2 = -1/\ln|\lambda^{(2)}|}$$

Master equation for Markov chains

$$p_i(t+1) = \sum_j W_{ij}\, p_j(t) + p_i(t) - p_i(t) \underbrace{\sum_j W_{ji}}_{=1}$$

$$= p_i(t) + \sum_j \left[W_{ij} P_j(t) - W_{ji} p_i(t) \right]$$

$$\underbrace{p_i(t+1) - p_i(t) = \sum_{j \neq i} \left[\underbrace{W_{ij} P_j(t)}_{\text{gain term}} - \underbrace{W_{ji} p_i(t)}_{\text{loss term}} \right]}_{\text{MASTER EQUATION}}$$

STATIONARITY $\iff \forall i \sum_{j \neq i} [W_{ij} p_j - W_{ji} p_i] = 0$

$(p_i(t+1) - p_i(t) = 0)$

DETAILED BALANCE $\iff \boxed{W_{ij} p_j = W_{ji} p_i}$ $\forall i \neq j$

D.B $\implies$ stationarity

$\cancel{\impliedby}$

D.B $\iff$ reversibility

$\downarrow$

Time reversal invariance

$\downarrow$

prob. forw. trajectory = prob. backward traj.

(same dynamical rules $\to$ same W)

MC satisfies DB

&

REVERSIBLE MC

Forward trajectory: $0 \quad 1 \quad 2 \quad \dots \quad n$ time

$S_{i_0} \quad S_{i_1} \quad S_{i_2} \quad \dots \quad S_{i_n}$ state

$$p\left(x(n) = S_{i_n};\ x(n-1) = S_{i_{n-1}}, \dots, x(1) = S_{i_1};\ x(0) = S_{i_0}\right)$$

$$\|$$

$$\underbrace{p_{i_0} \cdot W_{i_1 i_0}} \cdot W_{i_2 i_1} \cdots W_{i_n i_{n-1}}$$

stationary distrib. for which D.B. holds

$\xrightarrow{DB} W_{i_0 i_1} p_{i_1} \xrightarrow{DB} W_{i_1 i_2} p_{i_2}$

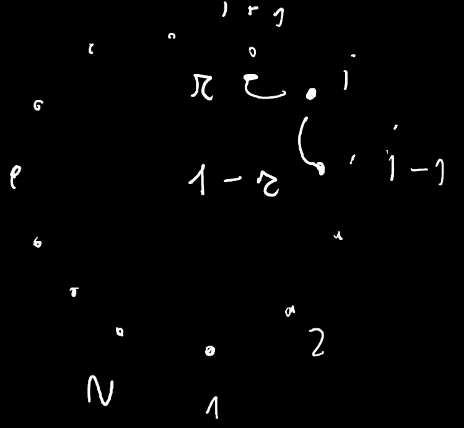
$$= W_{i_0 i_1} W_{i_1 i_2} \cdots W_{i_{n-1} i_n} \cdot p_{i_n}$$

$$\underbrace{P\left(X(n)=S_{i_0},\ X(n-1)=S_{i_1},\ \dots,\ X(0)=S_{i_n}\right)}_{\text{Prob. backward trajectory}}$$

$$\boxed{\begin{array}{l}\underline{\text{D.B.}} \longmapsto \text{equilibrium} \left(\begin{array}{c}\text{microscopic}\\ \text{reversibility}\end{array}\right) \\ \text{stronger condition than STATIONARITY}\end{array}}$$

MC example: Random Walk on a ring

(1d)



N states

$$W_{i+1,i} = r \ , \quad W_{i-1,i} = 1-r$$

$$W_{i,j} = 0 \text{ otherwise } (W_{ii} = 0)$$

Periodic Boundary Conditions (state $N+1$ = state 1)

$r = 1/2 \longrightarrow$ symmetric (unbiased) RW

$r \neq 1/2 \longrightarrow$ asymmetric (biased) RW

$$\underline{0 \le r \le 1}$$

Stochastic Matrix

$$W = \begin{pmatrix} 0 & 1-r & 0 & 0 & 0 & \cdots & r \\ r & 0 & 1-r & 0 & \cdots & \cdots & 0 \\ 0 & r & 0 & 1-r & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & 1-r \\ 1-r & \cdots & \cdots & 0 & r & & 0 \end{pmatrix}$$

Stochastic update rule:

$$p_i(t+1) = (1-\tau)\, p_{i+1}(t) + \tau\, p_{i-1}(t)$$

Stationary distribution $\hat{p}_i$

$$\rightarrow \quad \hat{p}_i = (1-\tau)\hat{p}_i + \tau \hat{p}_i \quad \forall i$$

Obvious solution $\hat{p}_i = 1/N \qquad \left(\sum_{i=1}^{N} \hat{p}_i = 1 \right)$

Spectrum of W: $\qquad W \bar{w} = \lambda \bar{w}$

eigenvalue problem: $\underbrace{(1-\tau)\, w_{k+1} + \tau\, w_{k-1} = \lambda w_k}$

Ansatz for the solution $\underbrace{w_k = \omega^k}$

ω determined by PBC $\rightarrow \underbrace{w_{N+1} = w_1}$

$$\rightarrow \underbrace{\omega_j = \exp\left(\frac{2\pi i}{N} j\right)} \quad \boxed{\omega^N = 1}$$

$j = 0, 1, \dots, N-1 \rightarrow j$ labels eigenvalues eigenvectors

eigenvalues $\lambda_j = (1-\tau)\, \omega_j + \tau \dfrac{1}{\omega_j}$

$$= \cos\left(\frac{2\pi j}{N}\right) + i(1-2\tau)\sin\left(\frac{2\pi j}{N}\right)$$

$\underline{\underline{\tau = 1/2}} \qquad \lambda_j = \cos\left(2\pi j/N\right) \in \mathbb{R} \quad (W_{ij} = W_{ji})$

$r \neq 1/2$ $\qquad \underbrace{\lambda_0 = 1}$ $\qquad$ eigenvector $(1, w_j, w_j^2, \dots, w_j^N)$

$\lambda_j \in \mathbb{C}$ $\qquad \longrightarrow \vec{W}^{(0)} = (1, 1, \dots, 1)$

for $j \geq 1$ $\qquad w_0 = 1$ $\qquad \Downarrow$

$(W_{ij} \neq W_{ji})$ $\qquad$ stationary distrib.

$r = 1/2 \longrightarrow$ D.B holds $\quad \hat{p}_i W_{ji} = \hat{p}_j W_{ij}$

$(\hat{p}_i = 1/N$ and $W_{ij} = W_{ji})$

$\longrightarrow$ NO CURRENT IN THE SYSTEM

zero average velocity

$\boxed{r \neq 1/2} \longrightarrow$ NO D.B. $\quad p_i W_{ji} \neq p_j W_{ij}$

$(\hat{p}_i = 1/N \; ; \; W_{ij} \neq W_{ji})$

STATIONARITY

BUT NO EQUILIBRIUM

$$\underset{\text{average velocity}}{v} = (+1) r + (-1) \cdot (1-r) = 2r - 1 \begin{cases} > 0 & r > 1/2 \\ = 0 & r = 1/2 \\ < 0 & r < 1/2 \end{cases}$$

CURRENT FLOWING IN THE SYSTEM

PROBLEMS WITH CONVERGENCE

Period 2 $\longleftarrow$ $\boxed{N \text{ even}}$

$$p_i(t) \xrightarrow[t \to \infty]{} 1/N \; (= \hat{p}_i)$$

does NOT hold for all initial conditions

(for example with $p_i(0) = \delta_{i,1}$)

$$\lambda_{N/2} = -1 \rightarrow \vec{w}^{(N/2)} = (1, -1, +1, -1, \dots)$$

weak convergence $\lim_{t \to \infty} \frac{1}{t} \sum_{1}^{t} z_i\, p_j(z_i) = 1/N$