Markov Chains

$\vec{x}$: states of a system, discrete, finite in number

t : discrete "time"

$$\vec{x}(t=0) \xrightarrow[\text{transition}]{\text{Stoch.}} \vec{x}(t=1) \longrightarrow \vec{x}(t=2) \longrightarrow \dots$$

Markov property: Transition probability depends only on the initial state, but not on the past.

homogeneous Markov chain:

transition probabilities do not explicitly depend on time.

$\underbrace{w(\bar{x} \to \bar{y})}$: probability to go from $\bar{x}$ to $\bar{y}$

$$0 \leq w(\bar{x} \to \bar{y}) \leq 1$$

$$\sum_{\bar{y}} w(\bar{x} \to \bar{y}) = 1$$

$P(\bar{x}, t)$: probability for the system to be at $\bar{x}$ at time t

Master equation:

$$P(\vec{x}, t+1) = P(\vec{x}, t) + \sum_{\vec{y}(\neq \vec{x})} w(\vec{y} \to \vec{x})\, P(\vec{y}, t)$$

$$- \sum_{\vec{y}(\neq \vec{x})} w(\vec{x} \to \vec{y})\, P(\vec{x}, t)$$

Now $P(\vec{x}, t)\left[1 - \sum_{\vec{y}(\neq \vec{x})} w(\vec{x} \to \vec{y})\right]$

$$= P(\vec{x}, t)\left[\sum_{\vec{y}} w(\vec{x} \to \vec{y}) - \sum_{\vec{y}(\neq \vec{x})} w(\vec{x} \to \vec{y})\right]$$

$$= P(\vec{x}, t)\, w(\vec{x} \to \vec{x})$$

$$\boxed{P(\vec{x}, t+1) = \sum_{\vec{y}} w(\vec{y} \to \vec{x})\, P(\vec{y}, t)}$$

new notation:

$$w(\vec{x} \to \vec{y}) =: w_{ij} \qquad i \mathrel{\hat{=}} \vec{x} \quad j \mathrel{\hat{=}} \vec{y}$$

initial final

$$P_i(t+1) = \sum_j w_{ji} \quad P_j(t)$$

$$\boxed{\vec{P}(t+1) = W^T \vec{P}(t)} \qquad \vec{P}(t) = (W^t)^T \vec{P}(0)$$

transposed matrix

Stationary distribution:

$$P(\vec{x}, t+1) = P(\vec{x}, t) = P_{stat}(\vec{x})$$

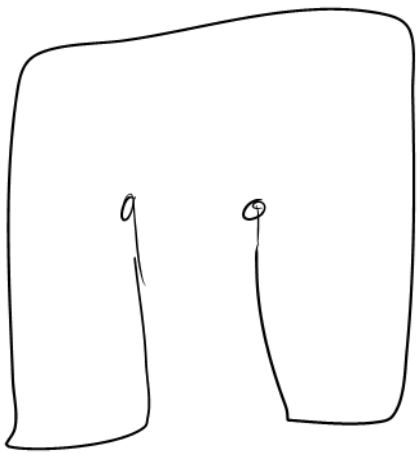
$$\vec{P}_{stat} = \bar{W}^T \vec{P}_{stat} \Rightarrow \vec{P}_{stat} \text{ is an eigenvector of } \bar{W}^T\text{, eigenvalue is ONE.}$$

Questions:

(i) $\vec{P}(t) \xrightarrow[??]{t \to \infty} \vec{P}_{stat}$

(ii) $\bar{W}^t \xrightarrow{t \to \infty} ??$

Definition: A Markov chain is called ERGODIC if each state can be reached from each other state, in a finite number of steps, with a finite probability.



In other words: There is an $L \geq 1$ <u>and</u> there is a $\delta > 0$: $(W^L)_{ij} \geq \delta$

for <u>all</u> pairs (ij)

<u>Ergodic Theorem by Markov</u>: If the chain is ergodic, then:

(i) There is ONE UNIQUE stationary distribution $\vec{P}_{stat}$, <u>and</u> $\vec{P}(t) \xrightarrow{t\to\infty} \vec{P}_{stat}$ regardless of the initial conditions,

(ii) $(W^t)_{ij} \xrightarrow{t \to \infty} P_{j\,stat}$

initial final

<u>Remark:</u>

$$P_i(t) = \sum_j (W^t)_{ji} \, P_j(0) \xrightarrow[\text{assume (ii)}]{t \to \infty}$$

$$\longrightarrow \underbrace{\sum_j P_j(0)}\, P_{i\,stat} = P_{i\,stat} \Rightarrow$$

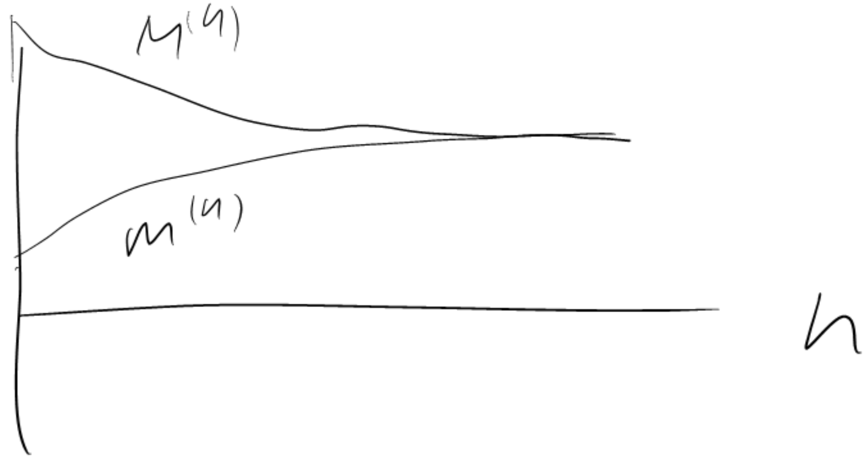
(ii) implies (i)

Proof: Let $w_{ij}^{(n)} = (\bar{W}^n)_{ij}$

and $m_j^{(n)} = \min_i w_{ij}^{(n)}$ $\quad M_j^{(n)} = \max_i w_{ij}^{(n)}$

study $m_j^{(n)}$, $M_j^{(n)}$ as a function of n

Show:



$$m_j^{(n+1)} = \min_i w_{ij}^{(n+1)} = \min_i \sum_k w_{ik} w_{kj}^{(n)} \geq$$

$$\geq \min_i \underbrace{\sum_k w_{ik}}_{1} m_j^{(n)} = m_j^{(n)}$$

$0 \leq m_j^{(n)} \leq 1 \longrightarrow m_j^{(n)}$ converges

Similar: $M_j^{(n)}$ decreases, converges.

Now study $M_j^{(n)} - m_j^{(n)}$ (≥ 0)

slow: $M_j^{(n)} - m_j^{(n)} \longrightarrow 0$ for $n \to \infty$

then we are DONE!

<u>Now</u> $M_j^{(n+L)} - m_j^{(n+L)} = w_{ij}^{(n+L)} - w_{kj}^{(n+L)}$

for some suitable i, k

Factorize this: $M_j^{(n+L)} - m_j^{(n+L)} =$

$$= \sum_{\ell} \left(w_{i\ell}^{(L)} w_{\ell j}^{(n)} - w_{k\ell}^{(L)} w_{\ell j}^{(n)} \right) =$$

$$= \sum_{\ell} \underbrace{\left(w_{i\ell}^{(L)} - w_{k\ell}^{(L)} \right)}_{\text{this is } \begin{cases} \geq 0 & \text{for } \ell \in I_+ \\ < 0 & \text{for } \ell \in I_- \end{cases}} w_{\ell j}^{(n)}$$

$$= \sum_{l\in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) \underbrace{w_{lj}^{(n)}}_{\le M_j^{(n)}} - \sum_{l\in I_-} \underbrace{\left(w_{kl}^{(L)} - w_{il}^{(L)} \right)}_{\geq 0} \underbrace{w_{lj}^{(n)}}_{\geq m_j^{(n)}} \le$$

$$\le \sum_{l\in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) M_j^{(n)} - \sum_{l\in I_-} \left(w_{kl}^{(L)} - w_{il}^{(L)} \right) m_j^{(n)}$$

$$= \sum_{l\in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) \left(M_j^{(n)} - m_j^{(n)} \right)$$

$$+ \sum_{l\in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) m_j^{(n)} + \sum_{l\in I_-} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) m_j^{(n)} =$$

$$= \underbrace{\sum_{l \in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right)}_{\text{some factor}} \underbrace{\left[M_j^{(n)} - m_j^{(n)} \right]} \geq M_j^{(n+L)} - m_j^{(n+L)}$$

if we can show that

$$\boxed{0 \leq \sum_{l \in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) \leq 1}$$

then $M_j^{(n)} - m_j^{(n)} \xrightarrow{n \to \infty} 0$ and we are done!

Study $\sum_{l \in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right)$

we know: $\sum_{l \in I_+} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) \geq 0$

$\hookrightarrow \sum_{l \in I_+} w_{il}^{(L)} \leq \sum_{l} w_{il}^{(L)} = 1$

$\hookrightarrow \sum_{l \in I_+} w_{kl}^{(L)} \geq \delta$ $\Big\{$ I_+ <u>cannot</u> be empty, since otherwise

$0 = \sum_{l \in I_-} \left(w_{il}^{(L)} - w_{kl}^{(L)} \right) < 0$ ↯ $\Big\}$

$$\Rightarrow 0 \leq \sum_{\ell \in I_+} \left(w_{i\ell}^{(L)} - w_{k\ell}^{(L)} \right) \leq 1 - \delta$$

theorem proven

<u>application</u>: construct $w(\bar{x} \to \bar{y})$ in such a way that $P_{stat}(\bar{x})$ is some <u>desired</u> distribution (<u>and</u> the chain is ergodic)

$\searrow$ Boltzmann

Master equation:

$$P_{stat}(\vec{x}) = P_{stat}(\vec{x}) + \sum_{\vec{y}(\neq \vec{x})} w(\vec{y} \to \vec{x})\, P_{stat}(\vec{y})$$

$$- \sum_{\vec{y}(\neq \vec{x})} w(\vec{x} \to \vec{y})\, P_{stat}(\vec{x})$$

$$\Big| + w(\vec{x} \to \vec{x})\, P_{stat}(\vec{x})$$

$$\sum_{\vec{y}} w(\vec{y} \to \vec{x})\, P_{stat}(\vec{y}) = \sum_{\vec{y}} w(\vec{x} \to \vec{y})\, P_{stat}(\vec{x})$$

stronger condition; detailed balance:

$$W(\vec{y} \to \vec{x})\, P_{stat}(\vec{y}) = W(\vec{x} \to \vec{y})\, P_{stat}(\vec{x})$$