Lecture October 29

PDF : $w_i(t)$ probability of being in a state $-i-$ at a time $-t-$

Normal situation : we have a model for $w_i(t)$.

P4 : $w_i(t) \longrightarrow P_i(T) = \dfrac{e^{-E_i/k_BT}}{Z}$

Z = normalization constant

$$Z = \sum_i e^{-E_i/k_BT}$$

Transition probability :

$W(j \to i)$ unknown

Markov chain

$$w_i(t+\varepsilon) = \sum_j \underbrace{W(j \to i)}_{\text{time independent}} w_j(t)$$

in equilibrium

$$\lim_{t \to \infty} \| w(t+\varepsilon) - w(t) \| = 0$$

$$\sum_i W_{ij} = 1$$

Example

$$W = \begin{bmatrix} 1/3 & 1/4 & 1 \\ 0 & 1/2 & 0 \\ 2/3 & 1/4 & 0 \end{bmatrix} \qquad \lambda = \{1, -2/3, 1/2\}$$

$$w(t+\varepsilon) = W\,w(t)$$

$\lim_{t \to \infty} w(t) \to w$

$$w = W \cdot w$$

Math of Markov chain

$W \in \mathbb{R}^{n \times n}$ has eigenvectors

$$W : \{v_1, v_2 \dots v_n\}$$

$$w(t=0) = w_0 = \sum_{i=1}^{n} a_i v_i$$

$$w(t=1) = w_1 = W w_0$$

$$= W \sum_{i=1}^{n} a_i v_i \qquad W v_i = \lambda_i v_i$$

$$= \sum_{i=1}^{n} \lambda_i a_i v_i$$

repeat m-times

$$w(t=m) = w_m = \sum_{i=1}^{n} \lambda_i^m a_i v_i$$

Example above

$$m = 100 \qquad \lambda_1 = 1 \quad \lambda_2 = -2/3$$
$$\lambda_3 = 1/2$$

$$w_{100} = 1^{100} a_1 v_1 + \overbrace{(-2/3)^{100}}^{10^{-18}} a_2 v_2$$
$$+ \underbrace{(1/2)^{100}}_{\simeq 10^{-31}} a_3 v_3$$

$$\simeq a_1 v_1$$

Example 2 + Metropolis

$$W = \begin{bmatrix} 3/4 & 1/2 \\ 1/4 & 1/2 \end{bmatrix} \qquad \lambda = \{1, 1/4\}$$

W = known

w = ?

$$w_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$w_1 = W \cdot w_0 = \begin{bmatrix} 0.6875 \\ 0.3125 \end{bmatrix}$$

$$\vdots$$

$$w_{17} \quad (W)^{17} w_0 = \begin{bmatrix} 2/3 \\ 1/3 \end{bmatrix}$$

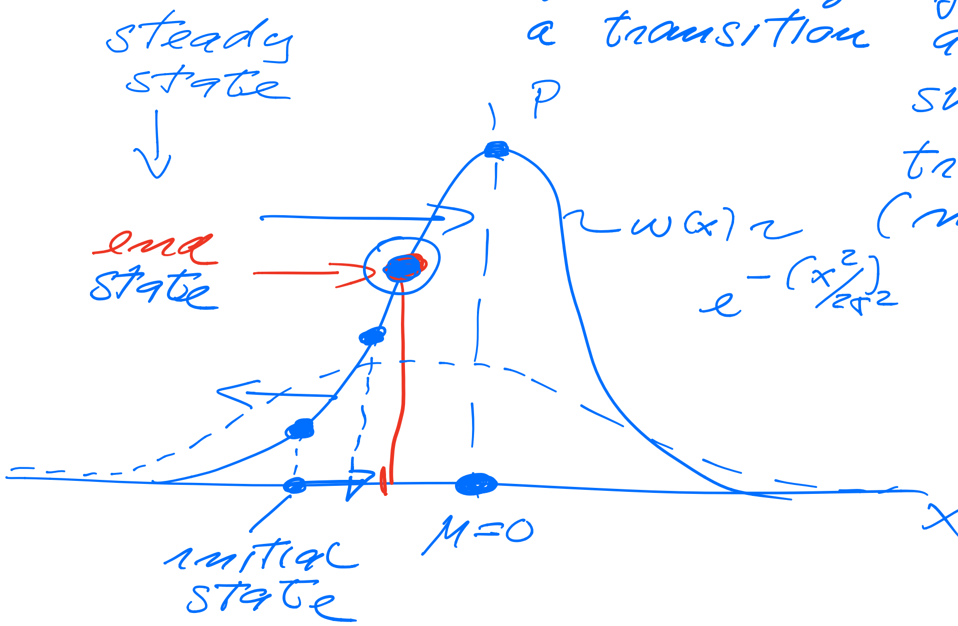
what if we know w but not W? The most common case.

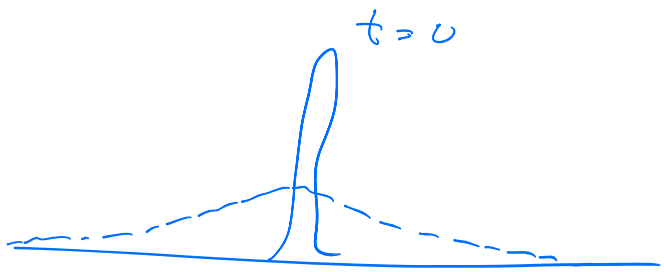
<u>Metropolis</u> saves the day

$$W(j\to i) = T(j\to i)\;A(j\to i)$$

likelihood for making a transition

likelihood for accepting suggested transition (move)





$$W_i^{(t+1)} = \sum_j \Big[W_j^{(t)}\, T(j\to i)\, A(j\to i) + W_i(t)\, \underline{T(i\to j)} \times \underbrace{\big(\underline{1} - A(i\to j)\big)}_{\text{net accept}} \Big]$$

$$\Big\{ \sum_j T(i\to j) = \sum_j T_{ij} = \underline{1} \Big\}$$

$$= \sum_j \Big[w_j^{(t)} T(j \to i) A(j \to i) - w_i(t) T(i \to j) A(i \to j) \Big]$$

$$+ w_i(t)$$

$$w_i(t+1) - w_i(t) =$$

$$\sum_j \Big[w_j(t) T(j \to i) A(j \to i) - w_i(t) T(i \to j) A(i \to j) \Big]$$

$$\lim_{t \to \infty} \| w_i(t+1) - w_i(t) \| = 0$$

$$w_i(t) \longrightarrow w_i$$

no time dependence

At most likely state:

$$\sum_j w_j T(j \to i) A(j \to i)$$

$$= \sum_j w_i T(i \to j) A(i \to j)$$

Detailed balance: For each j

$$\boxed{w_j T(j \to i) A(j \to i) = w_i T(i \to j) A(i \to j)}$$

Metropolis algo $\equiv$ sampling rule

$$\frac{w_i}{w_j} = \frac{e^{-E_i/k_BT}/Z}{\dfrac{e^{-E_j/k_BT}}{Z}} = e^{-(E_i-E_j)/k_BT}$$

we have a known model

Z = difficult to compute

$$Z = \sum_{i=1}^{M} e^{-E_i/k_BT}$$

N-spins (objects) $\Rightarrow$ 2^N configurations $= M$

$N = 100 \Rightarrow M = 2^{100}$

$$\boxed{\frac{w_i}{w_j} = \frac{T(j\to i)\,A(j\to i)}{T(i\to j)\,A(i\to j)}}$$

P4 symmetry $T(i\to j) = T(j\to i)$

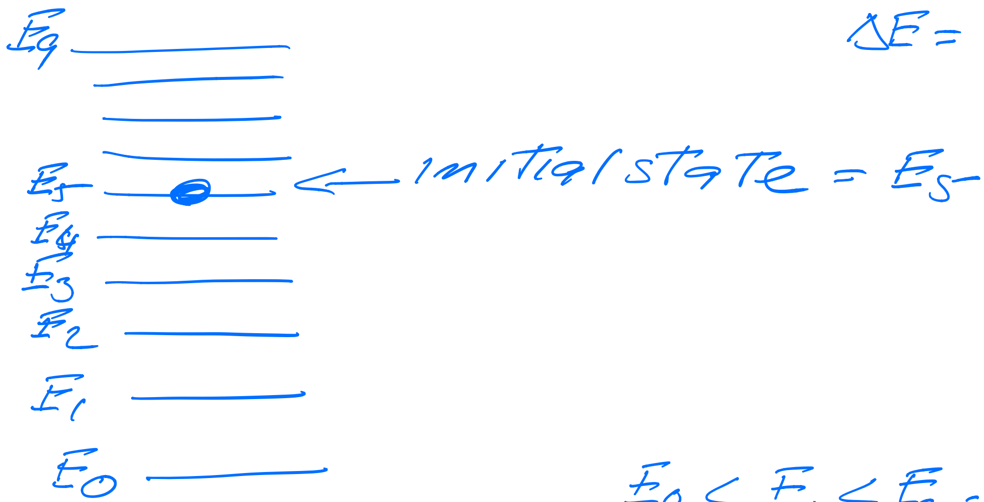
$$\frac{w_i}{w_j} = \frac{A(j\to i)}{A(i\to j)}$$

How do we model this?

$$0 \leq \frac{A(j \to i)}{A(i \to j)} \leq 1$$

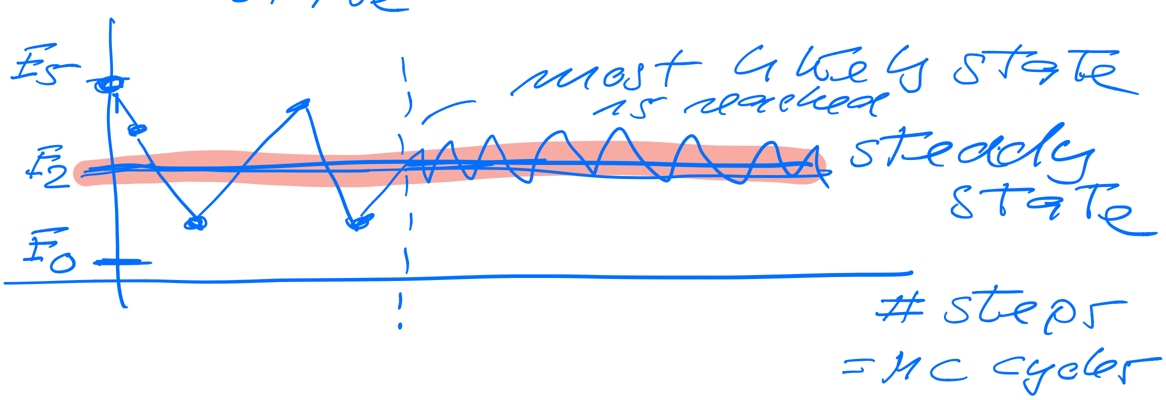
PU : $\dfrac{w_i}{w_j} = e^{-\beta \Delta E}$ $\qquad \beta = 1/k_B T$

$\Delta E = E_i - E_j$



$E_0 < E_1 < E_2 \ldots < E_9$

The steady state = E_2



First move : random choice = E_4

$\Delta E = E_4 - E_5 < 0$

Do we move to larger or

smaller probability

$$\frac{w_i}{w_j} = e^{-\beta(E_4 - E_5)}$$

$E_4 < E_5$ $\qquad$ $E_4 = 1$

$E_5 = 10$

$$e^{-10/\beta} \Rightarrow e^{-1/\beta}$$

P4 $\left[\frac{\text{Larger probability}}{\text{Lower energy}} \right|$ accept move.

$$\frac{w_4}{w_5} > 1 \qquad \frac{w_4}{w_4} = 1$$

$$e^{-\beta \Delta E} = \frac{A(j \to i)}{A(i \to j)}$$

Model our ignorance:

$w_i \geq w_j$ $\qquad$ ~~accept~~ set

$A(j \to i) = 1$

(max value)

$$0 \leq A(i \to j) < 1$$

$$w_i < w_j$$

$$\frac{w_i}{w_j} < 1 \quad \Rightarrow$$

$$\frac{A(j \to i)}{A(i \to j)} < 1 \quad \Rightarrow$$

$$A(j \to i) < A(i \to j)$$

set $A(i \to j) = 1$

$$\frac{w_i}{w_j} = A(j \to i) < 1$$

<u>algo</u>

$$A(j \to i) = \min\left(1, \frac{w_i}{w_j}\right)$$

pick $r \in [0, 1]$

$$\boxed{\text{if } r \le w_i / w_j \text{ accept}}$$

To compute

$\frac{w_i}{w_j}$ can be difficult.

– BAB

$e^{-\beta \Delta E}$ in p4 takes 5 values only, can pre-calculate.