FYS4411/9411 January 30

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PDF : $w(x,t)$

$$\left(w(x,t) \to P(\vec{R};\vec{\alpha}) = \frac{|\Psi_T(\vec{R};\vec{\alpha})|^2}{\int d\vec{R}\, |\Psi_T|^2} \right)$$

$$w(x, t=0) \to w(x,t)$$

steady state

Markov chain:

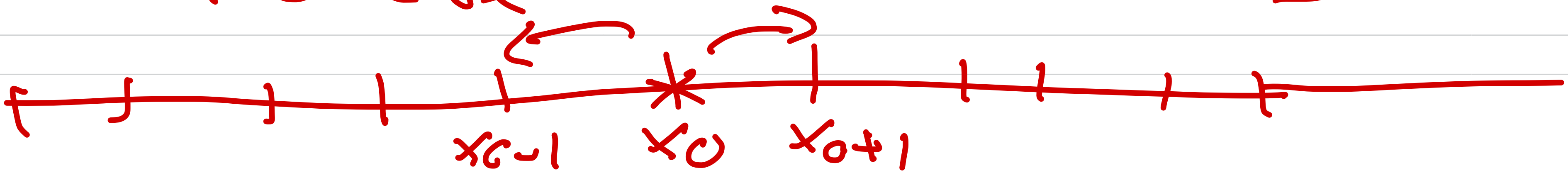
probability for being in a state i —

$w_i(t)$, after a step ε

$$w_i(t+\varepsilon) = \sum_j W_{ij}\, w_j(t)$$

Transition probability

$$W_{ij} = \begin{cases} \frac{1}{2} & \text{if } |i-j| = 1 \\ 0 & \text{else} \end{cases}$$ [unknown]



w_{ij} is an element of a stochastic matrix W

$$0 \leq w_{ij} \leq 1$$

$$\sum_j w_{ij} = 1$$

$$W = \begin{bmatrix} \frac{1}{2} & 0 & 1/3 \\ 1/4 & 0 & 1/3 \\ 1/4 & 1 & 1/3 \end{bmatrix}$$

$$|\lambda(W)| \leq 1$$

$$0 \le w_i \le 1$$

$$\sum_i w_i = 1$$

assumption: W is time independent

$$w_i(\varepsilon) = \sum_j W(j \to i)\, w_j(t=0)$$

$t = 0$

$$w(\varepsilon) = W w(0)$$

$$w(2\varepsilon) = W w(1) = W^2 w(0)$$

$$w(n\varepsilon) = W^n w(0)$$

W has eigenpairs (λ_i, v_i)

$$W v_i = \lambda_i v_i$$

$$w(0) = \sum_i \alpha_i v_i$$

$$W w(0) = \sum_i \alpha_i W v_i = \sum_i \alpha_i \lambda_i v_i$$

$$W^n w(0) = w(n) = \sum_i \alpha_i \lambda_i^n v_i$$

$$\varepsilon = 1$$

$$|\lambda(W)| \leq 1$$

$$|\lambda_0| \geq |\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$$

$$\tau_i = -\frac{1}{\log \lambda_i}$$

$$w(n) = \sum_{i=0}^{\infty} \alpha_i v_i e^{-n/\tau_i}$$

$$= \alpha_0 v_0 + \sum_{i=1}^{\infty} \alpha_i v_i e^{-n/\tau_i}$$

$$\lim_{n \to \infty} w(n) = \boxed{\alpha_0 v_0}$$

most likely state

Markov chain (steady state $n \to \infty$)

$$w(n) = W w(n)$$

$$\lambda = \underline{1}$$

$$w(n) \to w = W w$$

$$w_i(t) = \sum_j W(j \to i)\, w_j(t-1)$$

unknown

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

probability of making a transition

probability of acceptance

$$0 \leq T(j \to i) \leq 1 \qquad (T_{ij})$$

$$0 \leq A(j \to i) \leq 1 \qquad (a_{ij})$$

$$w_i'(t) = \sum_j W(j \to i)\, w_j(t-1)$$

accept j with probability $A(i \to j)$

probability of rejecting $(1 - A(i \to j))$

$$w_i(t) = \sum_j \Big[w_j(t-1)\, T(j \to i) \times A(j \to i) + w_i(t-1)\, T(i \to j) \times (1 - A(i \to j)) \Big]$$

when we reach the steady state

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

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

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

$$\sum_j w_i\, T(i \to j)\, \big(1 - A(i \to j)\big)$$

$$w_i - \sum_j w_i\, A(i \to j)\, T(i \to j)$$

$$\sum_j T(i \to j) = 1$$

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

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

$$\boxed{\begin{aligned} &w_j\, T(j \to i)\, A(j \to i) \\ &= w_i\, T(i \to j)\, A(i \to j) \\ &\text{Detailed balance} \end{aligned}}$$

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

Known since we have a model for w

$$w_i = P(\vec{R}_i ; \vec{\alpha}) = \frac{|\psi_T(\vec{R}_i ; \vec{\alpha})|^2}{N}$$

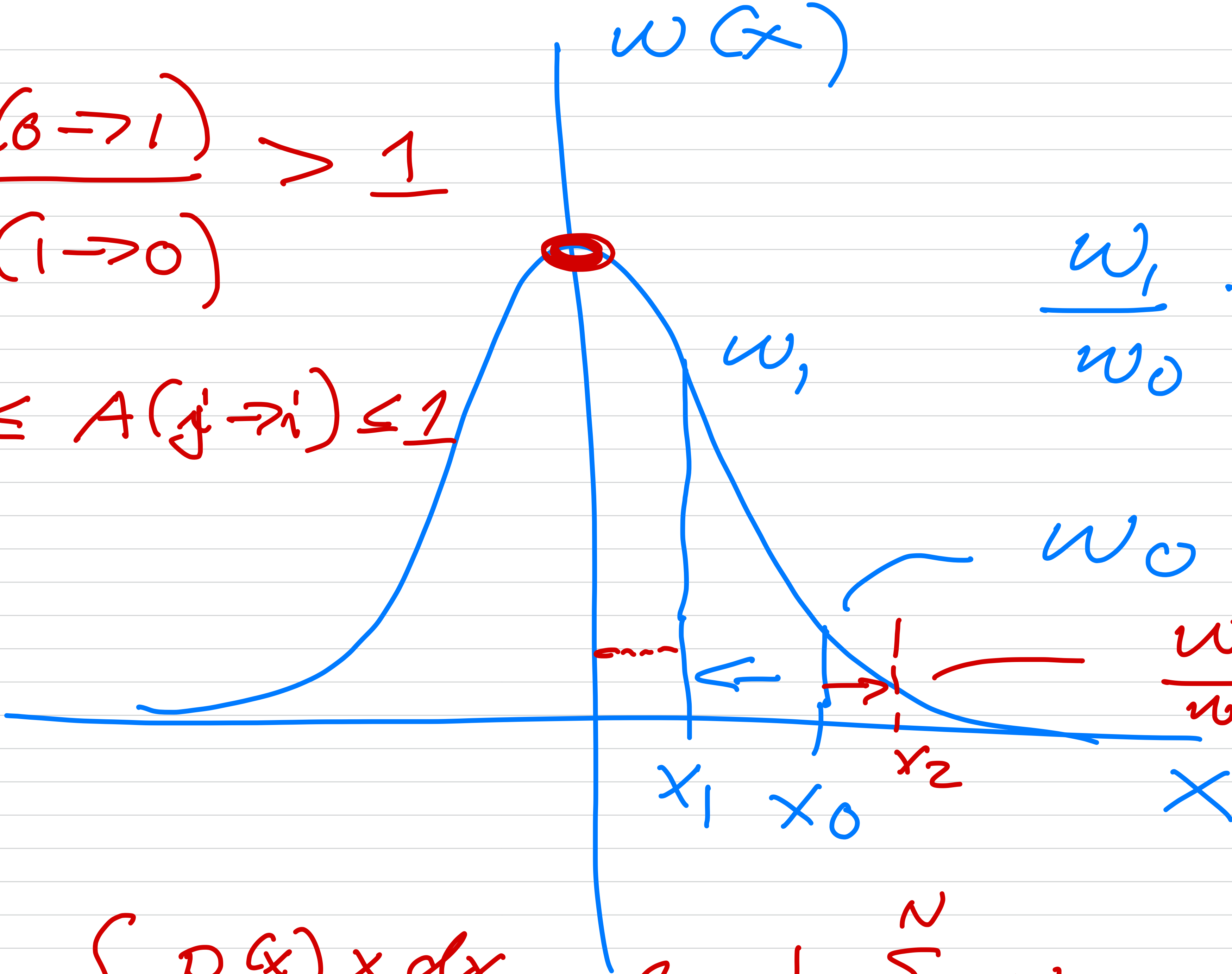
$$P(\vec{R}_i ; \vec{\alpha}) \sim e^{-\frac{1}{2}\alpha^2 x_1^2}\, e^{-1/2\, \alpha^2 x_2^2}$$

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

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

$$\frac{A(0\to 1)}{A(1\to 0)} > 1$$

$$0 \le A(j \to i) \le 1$$



$$\frac{w_1}{w_0} > 1$$

$$\frac{w_2}{w_0} < 1$$

$$\int p(x)\, x\, dx \approx \frac{1}{N} \sum_{i=1}^{N} x_i$$

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

Metropolis sampling

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

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

pick random number

$r \in [0, 1]$

if $r \leq w_i' / w_j'$, accept.

$$P_j(\beta) = \frac{e^{-\beta E_j'}}{Z}$$