FYS4411/9411
January 31

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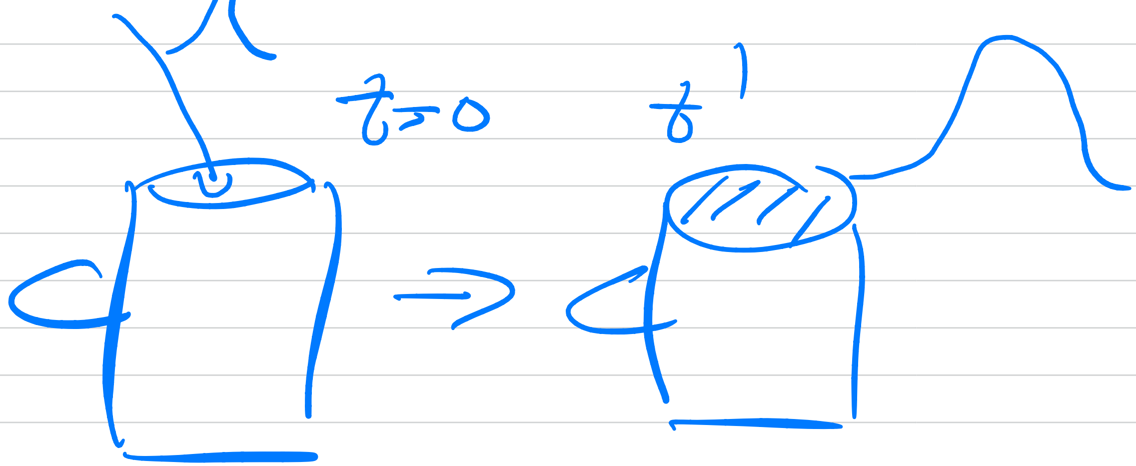
PDF : $w(x,t)$ $\left(P(\vec{R};\vec{\alpha}) = \dfrac{|\psi_T(\vec{R};\alpha)|^2}{\int |\psi_T(\vec{R};\alpha)|^2 d\vec{R}} \right)$

$w(x, t=0)$



$w(x, t=0) \rightarrow w(x,t) =$ steady state

Markov chain

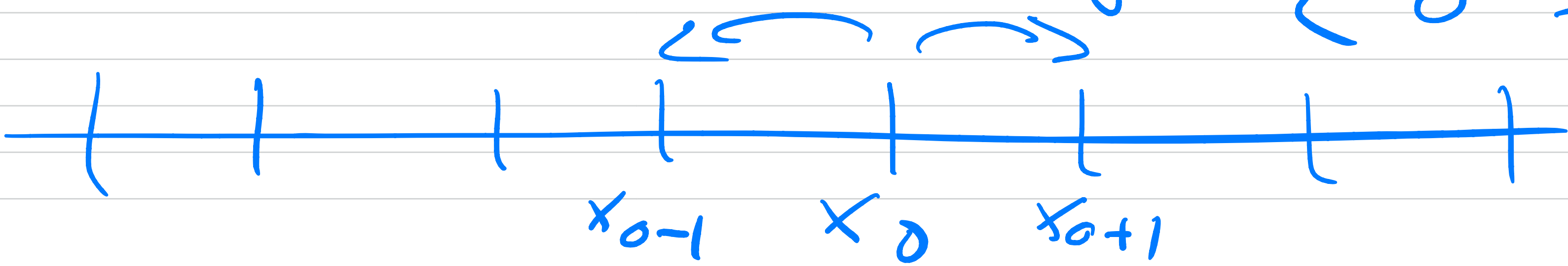
probability to be state -i- $w_i(t)$, after a step ε

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

unknown

Transition probability

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



$W_{ij} \rightarrow W$ is a stochastic matrix

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

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

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

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

$$0 \leq w_i \leq 1 \qquad \sum_i w_i = 1$$

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

$t=0$

assumption is W is time independent

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

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

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

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

W has eigenpairs (λ_i, v_i)

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

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

$$= \sum_i \alpha_i \lambda_i v_i$$

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

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

$$\lambda_0 = 0 \Rightarrow |\lambda_0| \geq |\lambda_n|$$

$$n \neq 0$$

$$n = 1, 2, \ldots N$$

$$\lambda_0 = 1 > \lambda_1 > \lambda_2 \ldots > \lambda_{N-1}$$

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

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

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

$$n\varepsilon = t$$

$$w(t) = \sum_i \alpha_i v_i e^{-t/\tau_i}$$

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

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

if we converge to the most likely state, then this corresponds to the largest eigenvalue ($\lambda_0 = 1$) of W with eigenvector $v_0 \cdot \alpha_0$

in this limit $w(t)$ becomes time independent

$$\underset{(=w(t))}{W w(t)} = \boxed{W w = w}$$

$\lambda = 1$

$$w_i(t+\varepsilon) = \sum_j \underbrace{\boxed{W(j\to i)}}_{\text{unknown}} \underbrace{\boxed{w_j(t)}}_{\substack{\text{known}\\ \text{model}}}$$

$W(j\to i)$ unknown

$$W(j\to i) = \underbrace{T(j\to i)}_{\substack{\text{Probability}\\ \text{to make}\\ \text{a transition}}} \underbrace{A(j\to i)}_{\substack{\text{probability}\\ \text{of}\\ \text{acceptance}}}$$

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

$$w_i(t) = \sum_j W(j \Rightarrow i)\, w_j(t-1)^{\varepsilon}$$

accept 'j' with probability $A(i \Rightarrow j)$, probability of rejecting $(1 - A(i \Rightarrow j))$

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

when equilibrium has been reached $w_i(t) = w_i(t-1)$

$$\left(\lim_{t \to \infty} w_i(t) = w_i \right)$$

$$\Rightarrow$$

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

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

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

$$= w_i \underbrace{\sum_j T(i \to j)}_{=1} - \sum_j w_i A(i \to j) \times T(i \to j)$$

Conditioned Balance

$$w_j' \, T(j \to i') \, A(j \to i')$$

$$= w_i' \, T(i' \to j) \, A(i' \to j)$$

$$\Rightarrow$$

$$\boxed{\frac{w_i'}{w_j'}} = \frac{T(j \to i') \, A(j \to i')}{T(i' \to j) \, A(i' \to j)}$$

known

$$w_i' \rightarrow P(\vec{R}_i'; \vec{\alpha}) = \frac{|\psi_T(\vec{R}_i; \vec{\alpha})|^2}{\int d\vec{R}\, |\psi_T|^2}$$

[stat mech

$w_i' \Rightarrow P_i'(T) = \dfrac{e^{-\frac{1}{k_B T} E_i'}}{\sum_i e^{-\frac{1}{k_B T} E_i'}}$

$$\frac{w_i'}{w_j'} = \frac{|\psi_T(\vec{R}_i; \vec{\alpha})|^2}{|\psi_T(\vec{R}_j; \vec{\alpha})|^2}$$

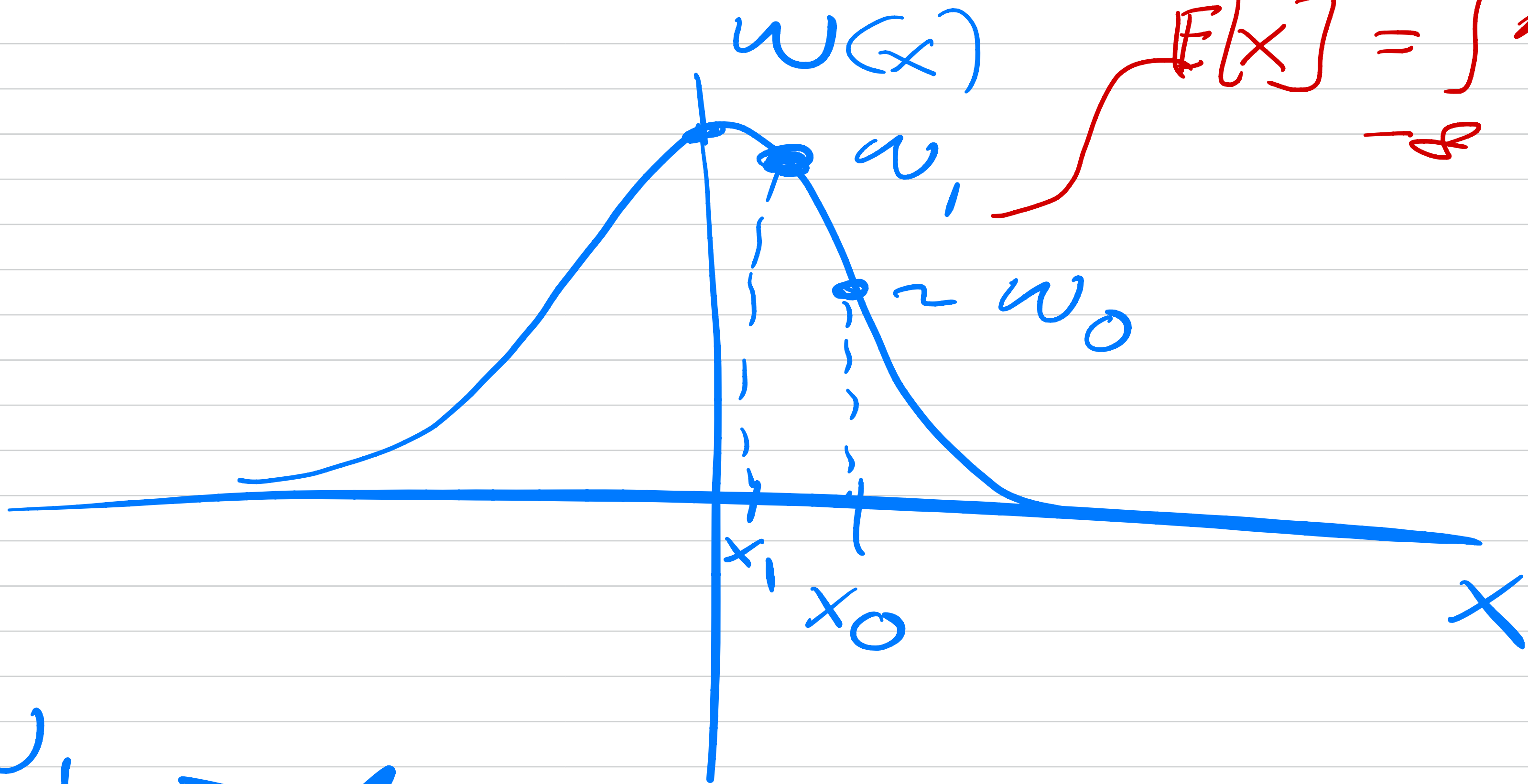
(i) Simple / Brute Force sampling

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

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

(if $T(i \to j) \neq T(j \to i)$ $\Rightarrow$ importance sampling)

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



$$E[x] = \int_{-\infty}^{\infty} w(x)\, x\, dx$$

$$\frac{w_1}{w_0} > 1 \Rightarrow \frac{w_i'}{w_j'} \geq 1$$

must also consider

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

Metropolis's choice

$$\frac{w_i}{w_j} > 1 \qquad \frac{A(j \to i)}{A(i \to j)} > 1$$

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

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

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

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

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

pick random number

$r \in [0,1]$

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