FYS4411 lecture, January 26, 2024

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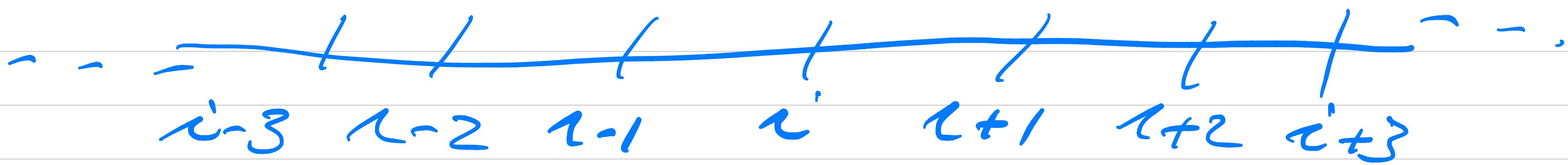
Markov chains & Metropolis algorithm

PDF : $w(x,t)$ $\quad | \quad |\psi(\vec{R};\alpha)|^2$

initial PDF $w(x,0) \rightarrow$

$w_i(0)$

Example $\qquad w_i(t)$



Markov chain

$$w_i(t+1) = w_i(t+\varepsilon)$$

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

Transition probability

simple W_{ij}

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

General case: We don't know W_{ij}

$w_{ij} \to W$ which is a stochastic matrix

$$0 \leq w_i \leq 1$$

$$\sum_{i=0}^{\infty} w_i(t) = 1$$

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

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

$$|\lambda(w_{ij})| \leq 1$$

$$\left. w_i(t+\varepsilon) \right|_{t=0} = w_i(\varepsilon) = \sum_j \underbrace{W(j\to i)}_{W_{ij}} \times w_j(0)$$

assumption W is time independent

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

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

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

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

W has eigenpairs (λ_i, v_i)

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

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

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

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

$$\lambda_0 = 1 > \lambda_1 > \lambda_2 > \dots > \lambda_{m-1}$$

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

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

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

$$n\varepsilon = t$$

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

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

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

stationary state / most likely state

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

time independent

Metropolis algorithm

$$W(j \to i) = ?$$

Make a model

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

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

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

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

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

$$= w_i(n-1) \quad \Rightarrow$$

$$w_i(n) = w_i(n-1)$$

$$+ \sum_j \Big[w_j(n-1)\,T(j \to i)\,A(j \to i)$$

$$- w_i(n-1)\,T(i \to j)\,A(i \to j) \Big]$$

$$\lim_{n \to \infty} w_i(n) = w_i'$$

stationary state

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

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

Detailed balance

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

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

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

known (we have a model for w_i)

Note: Normalization factor cancel

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

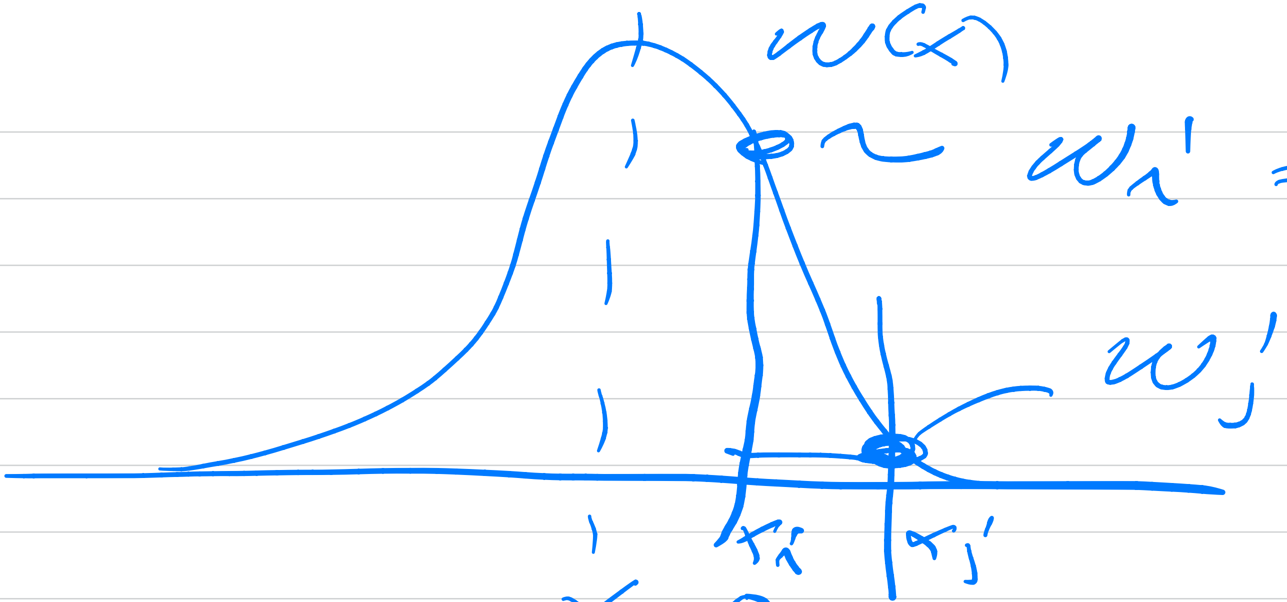
$$\frac{A(j \to i)}{A(i \to j)} = \frac{w_i \; T(i \to j)}{w_j \; \underline{T(j \to i)}}$$

specific for the given physics case

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

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

(Metropolis also)



$\sim \; w_i' = w(x_i')$

$x = 0$

$w_j = w(x_j)$

$$\frac{w(x_i')}{w(x_j')} = \, ?$$

$$\frac{w(x_i)}{w(x_j')} > 1 \quad \Bigg| \quad \frac{w(x_i')}{w(x_j')} = 1$$

$$\frac{w(x_i')}{w(x_j')} < 1$$

$$\frac{w(x_i)}{w(x_j)} \geq 1$$

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

$$\frac{w(x_i)}{w(x_j)} < 1$$

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

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

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

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

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

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

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