FYS 4411/9411 February 3, 2022

- Markov chain Monte Carlo
  $(MC)^2$

Discretized probability of being in a given state

- i -

$w_i(t)$

in our case

$$w_i(t) \to P_T(\vec{R}; \vec{\alpha})$$

$$= \frac{|\Psi_T(\vec{R}; \alpha)|^2}{\int_{\vec{R} \in D} d\vec{R} \, |\Psi_T(\vec{R}; \alpha)|^2}$$

$$\sum_{i \in \text{state}} w_i(t) = 1$$

Transition probability

$$W(j \to i) = W_{ij}$$

Markov chain

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

j

known (we have a model)

unknown

W is a stochastic matrix

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

$$w_i(t=0) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$W = \begin{bmatrix} 1/4 & 1/9 & 3/8 & 1/3 \\ 2/4 & 2/9 & 0 & 1/3 \\ 0 & 1/9 & 3/8 & 0 \\ 1/4 & 5/9 & 2/8 & 1/3 \end{bmatrix}$$

$$w(t=1) = W \cdot w(t=0)$$

$$= \begin{bmatrix} 1/4 \\ 1/2 \\ 0 \\ 1/ \end{bmatrix}$$

$$w(t=\infty) = \begin{bmatrix} 0{,}244 \\ 0{,}3196 \\ 0{,}057 \\ 0{,}379 \end{bmatrix}$$

Max eigenvalue $W = \underline{1}$
and represents the
so-called steady state

$$w(t) = W\, w(t-1)$$

lim $t \to \infty$ $\quad w(t=\infty) = W\, w(t=\infty)$

eigenvalue problem
with $\lambda = \underline{1}$

$$w(t) = W^{t}\, w(t=0)$$

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

eigenvectors of W

$$W v_i = \lambda_i v_i$$

$$w(t) = W^{t}\, w(t=0)$$

$$= W^{t} \sum_i \alpha_i v_i$$

$$= \sum_i \alpha_i v_i \lambda_i^{t}$$

λ_i : $\lambda_0 = 1 \geq \lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$

$$w(t) = \lambda_0^{t} \alpha_0 v_0 + \sum_{i=1}^{\infty} \alpha_i v_i \lambda_i^{t}$$

$$\lim_{t \to \infty} w(t) = \underset{\substack{\parallel \\ 1}}{\lambda_0} \alpha_0 v_0$$

Markov-chain Monte Carlo

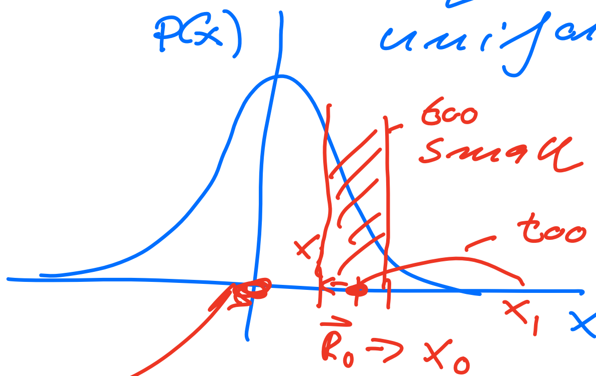
- initialize the system (initial positions $\vec{R}_0$)
- # attempted moves (# Monte Carlo cycles)
- Define $P_T(\vec{R}; \vec{\alpha})$

DO FOR $i = 1$, # Monte Carlo cycles

- suggest new position

$\bar{R} = \bar{R}_0 + RNG \times stepsize$

uniform distribution



$\int_{-\infty}^{\infty} p(x) \times dx$

$RNG \in [0,1]$
$= r$

$x_1 = x_0 + (r - 0.5) \times stepsize$

(i) wants to sample regions with large p(x)
if only this, then the contribution to

$$I = \int p(x)\, dx \times$$

will be biased

(ii) Allow jumping into regions with lower p(x).

→ sampling rule
= Metropolis algo

if position accepted

- update variables

else

stay in same place

previous value = new value

end loop

update averages

Sampling Rule = Metropolis - Hastings algo.

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

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

probability for making transition

Acceptance

probability

time independent

$$w_i'(t) = \sum_j \Big(w_j'(t-1)\, T_{j\to i} A_{j\to i} + w_i'(t-1)\, T_{i\to j} (1 - A_{i\to j}) \Big)$$

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

$$= w_i'(t-1) + \sum_j \Big[w_j'(t-1)\, T_{j\to i} A_{j\to i} - \underbrace{w_i'(t-1)\, T_{i\to j} A_{i\to j}} \Big]$$

$$w_i'(t) - w_i'(t-1) = \sum_j \Big[\qquad \Big]$$

$t \to \infty$

$$w_i'(t) = w_i'(t-1) \to$$

$w_i'(t) = w_i'$ time-independent

$$0 = \sum_j \Big[w_j' T_{j\to i} A_{j\to i}$$

$$w_i' T_{i\to j} A_{i\to j} \Big]$$

$$- w_i \, T_{i\to j} \, A_{i\to j} \Big]$$

$$\sum_{j} w_j \, T_{j\to i} \, A_{j\to i} = \sum_{j} w_i \, T_{i\to j} \, A_{i\to j}$$

Detailed balance

$$w_j \, T_{j\to i} \, A_{j\to i} = w_i \, T_{i\to j} \, A_{i\to j}$$

$$\frac{w_i}{w_j} = \frac{T_{j\to i} \, A_{j\to i}}{T_{i\to j} \, A_{i\to j}}$$

in our case

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

$$= \frac{T_{j\to i} \, A_{j\to i}}{T_{i\to j} \, A_{i\to j}}$$

importance sampling part.

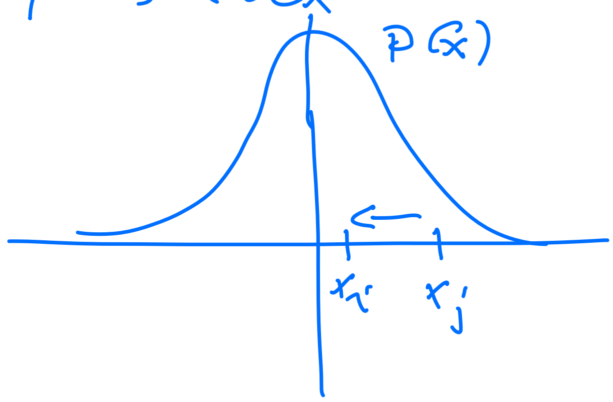
$$T_{i\to j} = T_{j\to i}$$

$$\frac{w_i}{w_j} = \frac{A_{j\to i}}{A_{i\to j}}$$

$$0 \le A_{i\to j} \le 1$$

(i) $\boxed{w_i \geq w_j}$ $\rightarrow$ $\frac{P(x_i)}{P(x_j)}$

$$\int_{-\infty}^{\infty} p(x)\, x\, dx$$



if $w_i \geq w_j$, accept move

$A_{j\to i}$

$$\frac{\cdots}{A_{i\to j}} \geq 1$$

$\boxed{\text{we set } A_{j\to i} = 1}$

its max value,

$A_{i\to j} \leq A_{j\to i}$

(ii) $w_i < w_j$

$$\frac{A_{j\to i}}{A_{i\to j}} < 1$$

$$A_{i\to j} = 1$$

$$A_{j\to i} < A_{i\to j}$$

Metropolis algo :

$$A_{j\to i} = \begin{cases} 1 & \text{if } w_i \geq w_j \\ \frac{w_i}{w_j} & \text{else} \end{cases}$$

$$= \min\left\{ \frac{w_i}{w_j}, 1 \right\}$$

implementation :

$$w_j = \left| \psi_T(\vec{R}_j; \vec{\alpha}) \right|^2$$

$$w_i = \left| \psi_T(\vec{R}_i; \vec{\alpha}) \right|^2$$

if $r \leq w_i / w_j$

random number $\in [0, 1]$

new position is $\vec{R}_i$

update expectation values $E_L(\vec{R}_i)$, $E_L(\vec{R}_i)^2$

call to E-local function.

else

$$\vec{R}_i = \vec{R}_j$$

add $E_L(\vec{R}_j)$, not moving is also a measurement.

Metropolis - Hastings

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

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

we need a model for $T_{i \Rightarrow j}$

use link between diffusion equation and Markov chains