FYS4411/9411 FEB 9, 2023

IMPORTANCE SAMPLING

$(MC)^2$

METROPOLIS HASTINGS

- Detailed balance from Markov chain
- Probability $w_i(t)$

$$\sum_i w_i(t) = 1$$

- Transition probability

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

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

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

$$\lambda_{max}[W] = 1$$

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

assumed time-independent

$$w(t) = W w(t - \Delta t)$$

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

$$w(t=\infty) = \begin{bmatrix} 0.2490 \\ 0.3196 \\ 0.0570 \\ 0.3790 \end{bmatrix}$$

steady state

$$\lim_{t \to \infty} w(t) = W w(t-1)$$

$$w(t=\infty) = W w(\infty)$$

$$w(t) = W^t w(t=0)$$

$$w(t=0) = \sum_i \alpha_i' v_i'$$

$$W v_i' = \lambda_i' v_i'$$

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

$$= \sum_i W \alpha_i' v_i'$$

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

$$w(t) = W^t w(t=0)$$

$$= \sum \lambda_i^t \alpha_i' v_i'$$

$$\lambda_0 = 1 \geq \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n-1}$$

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

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

$$w_i(t) \longrightarrow P(\vec{R}; \vec{\alpha})$$

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

Metropolis–Hastings

$W(j \to i) = W_{ij}$ this is normally unknown.

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

probability of making a transition

probability of accepting a suggested move

Metropolis-Hastings ratio

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

normally unknown

Metropolis $T(j \Rightarrow i) = T(i \Rightarrow j)$

standard:

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

$$= \frac{A(j \Rightarrow i)}{A(i \Rightarrow j)}$$

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

$$\frac{w_i}{w_j} \geq 1 \qquad \boxed{A(j \Rightarrow i) = 1}$$

$$0 \leq \frac{w_i}{w_j} < 1 \qquad \begin{array}{l} A(i \Rightarrow j) = 1 \\ A(j \Rightarrow i) \in [0,1) \end{array}$$

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

$r \in [0,1]$

if $r \leq w_i/w_j$

new position $\vec{R}_i$

update $E_L(\vec{R}_i)$

$E_L^2(\vec{R}_i)$

else

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

add $E_L(\vec{R}_j)$, $E_L^2(R_j)$

not moving is also a measurement

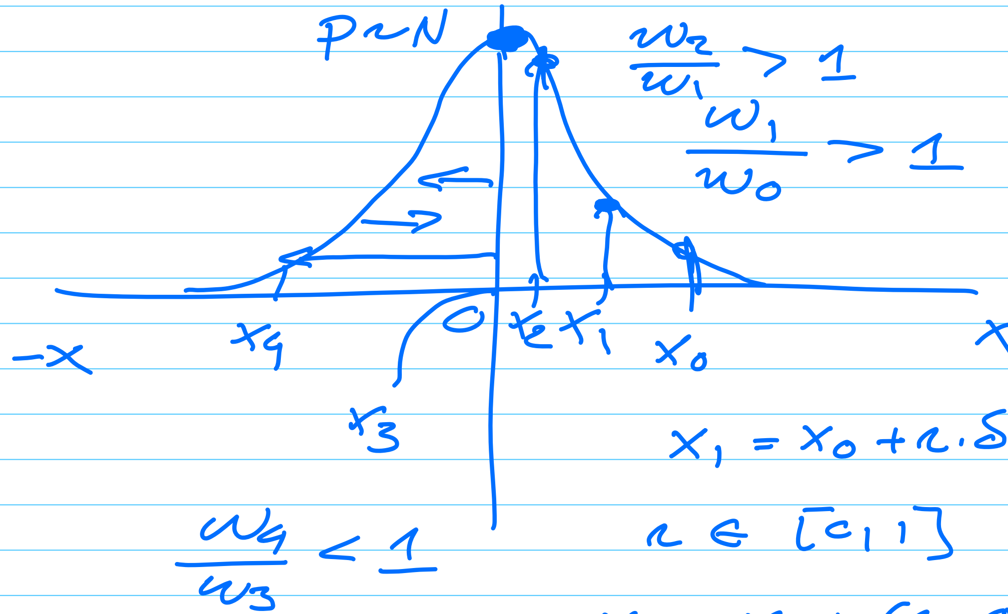
endif

Metropolis - Hastings

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

We need a model for $T(i \to j)$

Example $N(0,\sigma^2)$



$x_1 = x_0 + r \cdot \delta$

$r \in [0, 1]$

$x_1 = x_0 + (r - 0.5) \cdot \delta$

δ = chosen parameter

$$\langle x \rangle = \int_{x \in D} x \, p(x) \, dx$$

$$\simeq \frac{1}{N} \sum_{i=1}^{N} x_i$$

$\delta \Rightarrow$ importance sampling

Need a model for $T(i \Rightarrow j)$
Link with diffusion.

Discretized case:

$$w_i(0) \overset{\text{time } t_0 = 0}{=} \delta_{i,0}$$

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

Continuous choice

$$w_i(0) \Rightarrow w(\vec{x}, 0) = \delta(\vec{x})$$

Continuous Markov chain

$$w(\vec{y}, t+\Delta t) = \int_{x \in D} W(\vec{y}, \vec{x}, \Delta t) \times w(\vec{x}, t) \times d\vec{x}$$

in equilibrium

$$w(\vec{y}) = \int_{x \in D} W(\vec{y}, \vec{x})\, w(\vec{x})\, d\vec{x}$$

Fourier transform to k-space

$$w(\vec{x}, t) = \int_{-\infty}^{\infty} \exp(i\vec{k}\vec{x})\, \tilde{w}(\vec{k}, t)\, d\vec{k}$$

$$\delta(x) = \frac{1}{2} \int_{-\infty}^{\infty} \exp(i\vec{k}\vec{x})\, d\vec{k}$$

$$\tilde{w}(\vec{k}, 0) = 1/2\pi$$

Fourier-transform for Diffusion

$$\frac{\partial w(\vec{x},t)}{\partial t} = D\nabla^2 w(\vec{x},t)$$

$$\frac{\partial \tilde{w}(\vec{k},t)}{\partial t} = -D\vec{k}^2 \tilde{w}(k,t)$$

$$\tilde{w}(k,t) = \tilde{w}(\vec{k},0)\exp[-Dk^2t]$$

$$= \frac{1}{2\pi}\exp[-Dk^2t]$$

$$w(\vec{x},t) = \int_{-\infty}^{\infty} \exp(ikx)\frac{1}{2\pi}\exp[-Dk^2t] \times d\vec{k}$$

$$= \frac{1}{\sqrt{4\pi Dt}}\exp[-x^2/4Dt]$$

we can show that

$$W(\vec{y},\vec{x},\Delta t) =$$

$$\frac{1}{\sqrt{4\pi D\Delta t}}\exp\left[-(y-x)^2/4D\Delta t\right]$$

$$W(j \to i) = W(\vec{x} \to \vec{y}, \Delta t)$$

Solution for the diffusion equation for $W(j \to i)$

$$= W(\vec{x} \to \vec{y}, \Delta t) = W(\vec{y}, \vec{x}, \Delta t)$$

Metropolis - Hastings

$$\frac{w(\vec{y})}{w(\vec{x})} = \frac{A(\vec{x} \to \vec{y})\, W(\vec{y}, \vec{x}, \Delta t)}{A(\vec{y} \to \vec{x})\, W(\vec{x}, \vec{y}, \Delta t)}$$

$$\frac{W(\vec{y}, \vec{x}, \Delta t)}{W(\vec{x}, \vec{y}, \Delta t)} = 1$$

Need something different

$\Rightarrow$ Fokker - Planck eq.

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2}$$

+ Drift term.

modified $W(x, y, \Delta t)$

give model for $W(j \to i)$

$W(\vec{j} \to i)$ will be linked

with $|\psi_T(\vec{R}_i;\vec{\alpha})|^2$