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Metropolis-Hastings algorithm

- Detailed balance from a Markov chain

probability $w_i(t)$ known

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

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

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

transition probability

acceptance probability

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

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

$$T(i \to j) \neq T(j \to i) \Rightarrow$$

Metropolis - Hastings.

Link with Diffusion:

initial distribution

$$w_i(0) = \delta_{i,0}$$

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

Continuous choice

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

continuous Markov chain

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

<u>Equilibrium</u>

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

we can find $w(\vec{y},t)$ by 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-transformed diffusion

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

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

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

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

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

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

we can show that

$$W(\vec{y}, \vec{x}, \Delta t) = \frac{1}{\sqrt{4\pi D \Delta t}}$$

$$\times \exp\left[-(y-x)^2 / 4D\Delta t\right]$$

Metropolis-Hastings algo

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

$$T(i \to j) \propto \exp\left[-\frac{(y_i - x_j)^2}{4D\Delta t}\right]$$

Need a modification of the plain diffusion eq, Fokker-Planck eq.

$$q(y, x) = \frac{|\psi_T(y)|^2 \, G(y, x, \Delta t)}{|\psi_T(x)|^2 \, G(x, y, \Delta t)}$$

For systems with weak interactions, an independent particle model is a useful starting point.

For no interactions:

$$\Psi_T(\vec{R}) = \Psi_{Exact}(\vec{R})$$

$$\propto \prod_{i=1}^{N} \varphi_i(\vec{r}_i)$$

$$\hat{h}_i = -\frac{\hbar^2}{2m}\nabla_i^2 + V^{ext}(\vec{r}_i)$$

$$\hat{h}_i\,\varphi_\lambda(\vec{r}_i) = \varepsilon_\lambda\,\varphi_\lambda(\vec{r}_i)$$

$$\frac{|\Psi_T(\vec{R}_y)|^2}{|\Psi_T(\vec{R}_x)|^2} = \frac{\varphi_1^2(\vec{r}_{1y})\cdots\varphi_N^2(r_{Ny})}{\varphi_1^2(r_{1x})\cdots\varphi_N^2(r_{Nx})}$$

Two choices

1. move all particles and perform Metropolis test

2. move one particle at the time and perform the Metropolis test

- move 1 (first particle)

$$\frac{\varphi_1^2(\vec{r}_{1y})}{\varphi_1^2(\vec{r}_{1x})} \; \frac{\cancel{\varphi_2^2(\vec{r}_{2x})}}{\cancel{\varphi_2^2(\vec{r}_{2x})}} \; - - - \; \frac{\cancel{\varphi_N^2(\vec{r}_{Nx})}}{\cancel{\varphi_N^2(r_{Nx})}}$$

$$\Psi_T(\vec{R};\vec{\alpha}) = \prod_{i=1}^{N} \varphi_i(\vec{r}_i;\vec{\alpha}) \times \Psi_C$$

correlated part
Jastrow factor
contains the physics
of the interaction

$$\hat{V} = \sum_{i<j}^{N} \hat{v}(\vec{r}_{ij})$$

$$\vec{r}_{ij} = (\vec{r}_i - \vec{r}_j)$$

$$\hat{V}(\vec{r}_{ij}) \propto \frac{\gamma}{|\vec{r}_{ij}|}$$

$$\Psi_C = \prod_{i<j} g(r_{ij}) = \exp\left\{ \sum_{i<j} f(r_{ij}) \right\}$$

i

system dependent.