Mc Integral $\Rightarrow$ Markovian chain

类比从简→复. $x_1 \to x_2 \to x_3 \to \cdots \to x_n \to x_{n+1}$

$I = \int f(x)\, p(x)\, dx = \frac{1}{N} \sum_i f(x_i) \pm \delta I \qquad \delta I = \frac{\sigma}{\sqrt{N}}$ $\Rightarrow$ 高维: Euler差分

$O(N^{-4/d})$

1) 产生一组数 $\{x_i\}$.

2) $\{x_i\} \to p(x)$

3) 平衡 ~ 收敛.

$\Rightarrow x_i \Rightarrow \vec{x}_i$

$d=1$ 推广至 d 维

$p(x) \to p(\vec{x})$

$f(\vec{x})$ 有明确的物理意义.

1) $f(\vec{x}) = e^{-\beta H(\vec{x})}$

积分 $I = \mathrm{Tr}\left(e^{-\beta H(\vec{x})}\right) = \int d\vec{x}\, e^{-\beta H(\vec{x})}$ 高维积分.

Ising model.

2) Path Integral Mc.

Ising Model.

Ising 证明.

$H = -J \sum_i \sigma_i \sigma_{i+1}$ 无相变

$\sigma_i = \pm 1$. 转移矩阵.

Heisenberg Model.

$H = -J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$

1944 Onsager.

3d Ising Model. 至今未解决.

积分 $\{x_i\}$.

Metropolis 算法

Metropolis - Hasting

Gibbs

} 本节课不作区分

$\xi \in [0,1]$

$$x_{n+1} = \begin{cases} x^{new} & \xi < r = \min\{1, \frac{p(x^{new})}{p(x_n)}\} \\ x_n & \xi > r \text{ ，维持现状.} \end{cases}$$

→ Ising Model.

$$x_n \to \vec{x}_n \to \vec{\sigma} = \otimes Z_2^N = \underbrace{Z_2 \otimes Z_2 \otimes Z_2 \cdots}_{N = L^3}$$

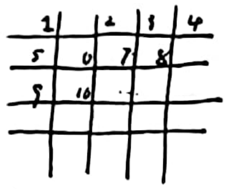
$$\vec{\sigma}_n \xrightarrow{\text{随机改变一个值}} \vec{\sigma}_{n+1}$$

$$m = \sum_{\{\sigma\}} m(\sigma) e^{-\beta H(\sigma)} / Z.$$

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j .$$

算法: 1) 初始化 $\sigma = (\sigma^1, \sigma^2, \cdots, \sigma^N)$

2) 随机找一个 $i \Rightarrow \sigma_n^i \to -\sigma_n^i$ } $\vec{\sigma}_n \to \vec{\sigma}_{n+1}$



产生格子(给出序号).
明确近邻关系.

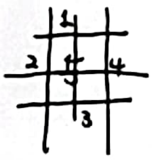
3) 计算 $r = \min\{1, \frac{p(x^{new})}{p(x_n)}\} \Rightarrow \Delta E$.

$$p(\vec{x}) = e^{-\beta H(x)} / Z$$

$$p(x^{new}) / p(x_n) = e^{-\beta(H(x^{new}) - H(x_n))} = e^{-\beta \Delta E}.$$

计算 $\Delta E = H(\vec{\sigma}_n') - H(\vec{\sigma}_n)$

$$= -2J \sum_{j \in \text{neighbor of } i} \sigma_n^i \sigma_n^j .$$



$\Rightarrow$ 前 $(\sigma_1\sigma_5 + \sigma_2\sigma_5 + \sigma_3\sigma_5 + \sigma_4\sigma_5)(-J)$

后 $\sigma_5 \to -\sigma_5 = \sigma_5'$

$(\sigma_1\sigma_5 + \sigma_2\sigma_5 + \sigma_3\sigma_5 + \sigma_4\sigma_5)(-J)(-1)$

$$\Delta E = 2J(\sigma_1\sigma_5 + \sigma_2\sigma_5 + \sigma_3\sigma_5 + \sigma_4\sigma_5)$$

④ $\vec{\sigma}_{n+1} = \begin{cases} \text{accept} = \vec{\sigma}' & \xi < r = \min\{1, e^{-\beta\Delta E}\} \\ \text{reject} = \vec{\sigma}_n & \text{other-wise.} \end{cases}$

计算 $Z = \mathrm{Tr}(e^{-\beta H})$

$\downarrow$

$Z = e^{-\beta F}$

F: Free energy $\rightarrow$ $-\dfrac{\partial \ln Z}{\partial \beta} = \langle H \rangle$

Ising Model. $H = -J\sum_{\langle ij \rangle} \sigma_i \sigma_j + \sum_i h\sigma_i \Rightarrow f(\vec{x}) = e^{-\beta H}$ $\quad \vec{x} = \vec{\sigma} = \{\sigma^1, \sigma^2, \cdots, \sigma^N\}$

$\sigma^i = \pm 1$

path Integral $H = -\frac{1}{2m}\frac{d^2}{dx^2} + V(\vec{R})$

$$Z = \int dR_0 \cdots dR_{n-1}\, e^{-H} = \int dR_0 \cdots dR_{n-1} f(\vec{R})$$

$$H = -\Delta\tau \sum_j \left[\frac{m}{2}\frac{(R_{j+1}-R_j)^2}{\Delta\tau^2} + V(R_j)\right]$$

Path Integral. MC.

$Z = \mathrm{Tr}(e^{-\beta H})$ 　　求 $V(\vec{x})$ 最小值.

$H = -\frac{1}{2m}\frac{d^2}{dx^2} + V(x)$ 　　$\lim\limits_{\beta\to 0} Z(\beta) = e^{-\beta E_g}$.

$$Z = \int dx \langle x| e^{-\beta H} |x\rangle$$

$$= \int dx_1 \cdots dx_{N-1} \langle x_1| e^{-\Delta t H} |x_1\rangle \langle x_1| e^{-\Delta t H} |x_2\rangle \cdots \langle x_{N-1}| e^{-\Delta t H} |x_1\rangle$$

计算 $\langle x_i | e^{-\Delta t (T+V)} | x_{i+1} \rangle$

$$= \langle x_i | e^{-\Delta t T} e^{-\Delta t V(x)} | x_{i+1} \rangle$$

$$= \langle x_i | e^{-\Delta t T} | x_{i+1} \rangle e^{-\Delta t V(x_{i+1})}$$

$\langle x| e^{-\Delta t T} |y\rangle$ 　　$\langle x| e^{-\Delta t T} |y\rangle$

$$= \int \langle x| e^{-\Delta t T} |k\rangle \langle k|y\rangle dk = \int dk\, e^{-\frac{m}{2}\Delta t k^2 + ik(x-y)}$$

$T = \dfrac{m(y-x)^2}{2\Delta t^2}$ 　　$T = -\frac{m}{2}\frac{d^2}{dx^2}$ 　$T|k\rangle = \frac{m}{2}k^2|k\rangle$ 　　$= e^{-\frac{1}{2m}\left(\frac{y-x}{\Delta t}\right)^2}$

总结：

$$I = \int f(\vec{x})\, p(\vec{x})\, d\vec{x} = \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)$$

应用：① 积分：

② $f \sim e^{-\beta H}$，H. energy Hamiltonian.

1) Ising Model.

2) Path Integral MC of H.

③ 求 $\vec{V}(\vec{x})$ 极值 (kinetic MC)

中心1. 大数：

1) 随机一维扩散定理：$\langle x^2 \rangle = 2Dt$.

2) Ito - lemma.

3). MC simulation. $\delta I = \frac{\sigma}{\sqrt{N}}$ ~ 差分. $N^{-4/d}$

作业

1) 求高维积分.

2) 产生任何一个 $p(x)$ 分布.

3) 求 2d, 3d Ising Model 的相变.