- MCMC产生任意 $P(x)$ 及MC统计 (PPT)

产生一组 $P(x_i)$ 分布的随机数

马尔可夫链 $P(x^{i+1}|x^i x^{i-1} \dots x^1) = P(x^{i+1}|x^i)$

Metropolis 算法

$$x^{i+1} = \begin{cases} x^{new} & p = r \\ x^i & p = 1-r \end{cases} \qquad r = \frac{P(x^{new})}{P(x^i)}$$

$r \geq 1$，完全接受 $x^{i+1} = x^{new}$ $\quad x^1 \to x^2 \cdots x^K$ $\quad K$ 足够大，满足平衡分布

考虑 $$\frac{dP_n}{dt} = \sum_m \underbrace{P_m W_{m\to n} - P_n W_{n\to m}}_{= 0}$$

0，细致平衡

tips

$\pi/4$ × $\quad 0.25\pi$ ✓ $\quad$ 循环里的常数 (π * π 之类) 放在外面算

作业 2D Ising 的相变 (见下)

- 重要抽样

均匀分布 $\langle f \rangle = \dfrac{\int p(x) f(x) dx}{\int p(x) dx = 1} = \frac{1}{N}\sum_i f(x_i)$

$g(x)$ 分布 $\quad \frac{1}{N}\sum_i \frac{f(x_i)}{g(x_i)} = \int f(x) dx$

- 2d Ising

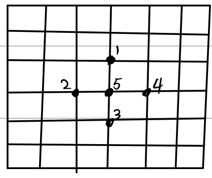
$$H = -J \sum_{ij} s_i s_j \quad (s_i = \pm 1)$$

$100 \times 100 \qquad |K| = 2^{10^4}$

$$x^{k+1} = \begin{cases} x^{new} \\ x^k \end{cases} \quad \cdots \qquad X^k \to S_i$$

高维 X 如何产生？

$$r = P(x^{new})/P(x^k) = e^{-\beta(E(x^{new}) - E(x^k))}$$



$E^{new}-E^{k}=-J(S_1+S_2+S_3+S_4)S_5$

相变点附近涨落大，翻转多，MC可能不精确

翻转 $J(S_1+S_2+S_3+S_4)S_5$

$$\langle m\rangle = \frac{\sum m(S)\, e^{-\beta H(S)}}{Z} = \frac{1}{N}\sum m(S_i)$$

$$\chi \propto \langle m^2\rangle - \langle m\rangle^2$$

χ怎么过渡到$S_1, S_2 \cdots S_n$

· 转移矩阵方法（1d为例）

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

$$Z = \sum_{\{\sigma_i\}} e^{\beta J\sum\sigma_i\sigma_{i+1} + \beta h\sum_i\sigma_i}$$

$$= \sum_{\{\sigma_i\}} P_{\sigma_1\sigma_2}P_{\sigma_2\sigma_3}\cdots P_{\sigma_N\sigma_1} = \mathrm{Tr}(P^N) = \mathrm{Tr}(U^{\dagger}\lambda^N U) = \mathrm{Tr}(\lambda^N)$$

$$P_{\sigma_1\sigma_2} = e^{\beta J\sigma_1\sigma_2 + \frac{\beta h}{2}(\sigma_1+\sigma_2)} \qquad \sigma_i = \pm 1$$

$$P = \begin{pmatrix} e^{\beta J+\beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J-\beta h} \end{pmatrix}$$

$$Z = e^{-\beta F} = \lambda_{max}^N = e^{N\ln\lambda_{max}}$$

$$\beta F = -N\ln\lambda_{max} \qquad \boxed{\beta f = -\ln\lambda_{max}}$$

作业1 讨论配函数性质

Onsager $F = -k_BT\ln Z$, $Z=\lambda^N$

$$\ln\lambda = \ln\left(2\cosh(2\beta J)\right) + \frac{1}{\pi}\int_0^{\pi}\ln\left[\frac{1}{2}\left(1+\sqrt{1-k^2\sin^2(\omega)}\right)\right]d\omega$$

$$k = \frac{2\sin(2\beta J)}{(\cosh(2\beta J))^2} \qquad \text{相变点：} k_BT_c = \frac{2J}{\ln(1+\sqrt{2})}$$

$$\begin{cases} E = -\dfrac{\partial\ln Z}{\partial\beta} \qquad Z = e^{\beta F} \\ C_v = \dfrac{\partial E}{\partial T} = \dfrac{\partial E}{\partial\beta}\dfrac{\partial\beta}{\partial T} = -\dfrac{1}{k_BT^2}\dfrac{\partial E}{\partial\beta} = -\dfrac{1}{k_BT^2}\left[\dfrac{1}{Z}\left(\dfrac{\partial Z}{\partial\beta}\right)\right] \end{cases}$$

$$-\frac{1}{k_B T^2}\left[-\underbrace{\frac{1}{Z^2}\left(\frac{\partial E}{\partial \beta}\right)^2}_{\Downarrow} + \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}\right]$$

$$\left(\frac{\partial \ln Z}{\partial \beta}\right)^2 = -E^2 = -\langle E\rangle^2$$

证明 $C_V \propto \left(\langle E^2\rangle - \langle E\rangle^2\right)$ 只要证明 $\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} = \langle E^2\rangle$

类比 $h \leftrightarrow \beta$, $h \downarrow m$, $\beta \downarrow E$

$$m = \frac{\partial \ln Z}{\partial h}$$

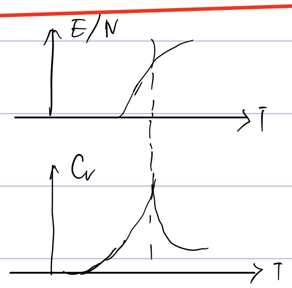
$$\chi = \frac{\partial m}{\partial h} \propto \langle m^2\rangle - \langle m\rangle^2$$

$$Z = \int e^{-\beta H} dx$$

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} = \int H^2 e^{-\beta H} dx / Z = \langle E^2\rangle$$

$\ln \lambda^N$

$$E = -N\frac{\partial \ln \lambda}{\partial \beta}$$



计算 $C_V \propto \frac{1}{|T-T_c|^\nu}$ 的 ν

$\ln C_V \propto -\nu \ln|T-T_c| + const$

Tips, 线性拟合

作业2