بسم الله الرحمن الرحیم

جلسه ۱۴۰۰/۱۰/۱۶

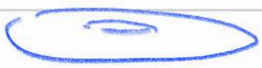
2-Dimensional Ising model

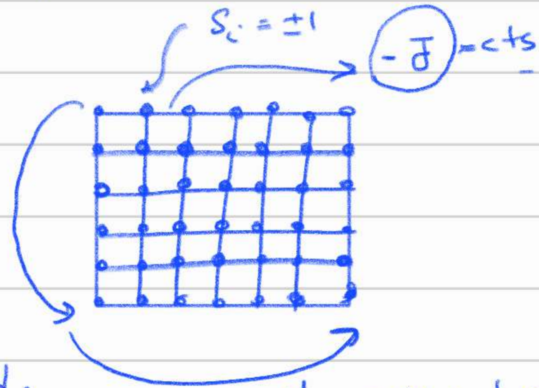
$$\langle f\rangle = \sum_i f_i\, p_i \longrightarrow \text{Importance Sampling}$$

- به جای اینکه همه پیکربندی‌ها را در نظر بگیریم صرفاً آن دسته از پیکربندی‌هایی را در نظر می‌گیریم که احتمال بیشتری رخ می‌دهند

2D-Ising model $\quad S = +1, -1$

MCMC Algorithm





Initial Condition

Construct a configuration for $\{S_i^{old}\}$ $\quad i=1, \; N_{spin} \equiv$ # nodes

Randomly Distributed Configuration

$$\mathcal{H}_{old} = -J \sum_{\langle ij\rangle} S_i^{old} S_j^{old} - B_{ext} \sum_{i=1}^{N_{spin}} S_i$$

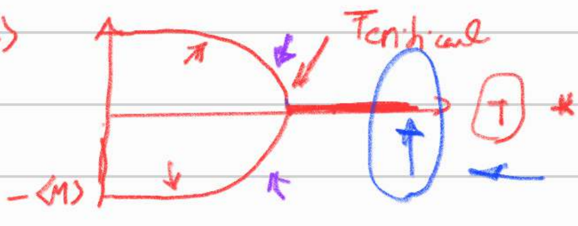
$$M_{old} = \sum_{i=1}^{N_{spin}} S_i^{old}$$

A $\quad \Delta E(\phi, P)$ s ✓

یادآوری

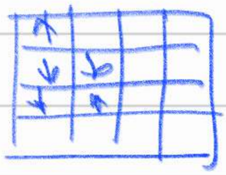
Second order Phase transm $\longrightarrow$ Magnetic System

Ferromagnetic System



$-J\, S_i S_j$ $\quad J>0$

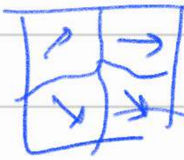
loop on T (High — low)



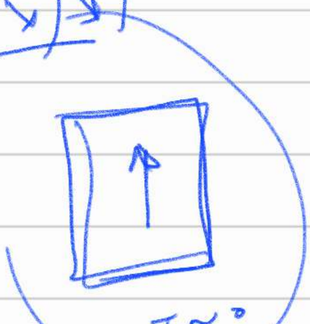
T ↗

Mean-Mag = 0

Mean-Energy = 0



loop on MCMC $v = 1, M$



T ~ 0

loop $i = 1, N_{spin}$

Select S_i^{old} Randomly and do

$\{ S_i^{old} \longrightarrow S_i^{New} = -S_i^{old} \}$

کپی کن → $S_i' = S_i^{old}$

$S_i^{New} = -S_i^{old}$ [illegible]

spin flip

$S(x,y)^{old} =$ ✓

Sum = S(x-1,y) + S(x+1,y) + S(x,y+1) + S(x,y-1)

$q = +2\,\text{Sum}\,S_i^{old}$, $p = +2 S_i^{old}$

$\Delta E(\beta, p) =$ subroutine ΔE

$\mathcal{H}_{New} = \mathcal{H}_{old} + \Delta E$

$e^{-\beta\mathcal{H}}$ Prior

R = call Random Number

$R = \min\{1, \frac{P_{New}}{P_{old}}\}$

if $R \leqslant e^{-\beta\Delta E}$

$\frac{e^{-\beta\mathcal{H}_{New}}}{e^{-\beta\mathcal{H}_{old}}}$

Importa

Metropolis Part

$\mathcal{H}_{old} = \mathcal{H}_{New}$

$S_i^{old} = S_i^{New}$

End if

Canonical Ensem

$\sim M(\nu) = \left| M_{old} - S_i' + S_i^{old} \right|$

End loop N_{sph}

→ Mean_Mag = Mean-Mag + $M(\nu)$

→ $\mathcal{H}(\nu) = \mathcal{H}_{old}$

→ Mean_Energy = Mean_Energy + $\mathcal{H}(\nu)$

End loop MCMC

Var_mag = 0

Var_energy = 0

loop $\nu = 1$, MCMC

Var_mag = Var_mag + $(M(\nu) - \text{mean\_mag})^2$

Var_energy = Var_energy + $(\mathcal{H}(\nu) - \text{mean\_energy})^2$

End loop

Write T, mean_mag → T, $\langle M(T) \rangle$

write T, mean_energy → T, $\langle \mathcal{H} \rangle$

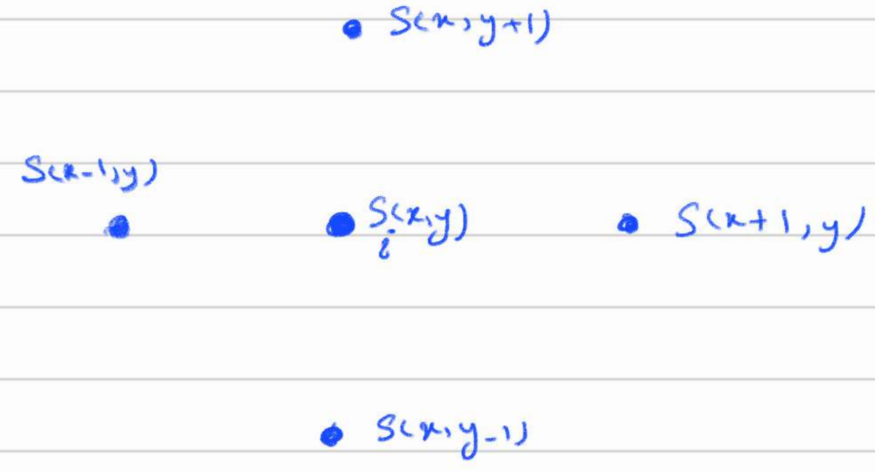
write T, $\dfrac{\text{Var\_mag}}{K_B T}$ → T, χ → σ_M^2

write T, $\dfrac{\text{Var\_energy}}{K_B T^2}$ → T, C_V → $\sigma_{\mathcal{H}}^2$

End T

Subroutine for Computing $\underline{\Delta E}$

①



②

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - B_{ext} \sum_{i=1}^{N_{spin}} S_i$$

$$\mathcal{H}_i = -J S_i \sum_{\langle j \rangle} S_j - B_{ext} S_i$$

$$= \Big[\underbrace{-J \sum_{\langle j \rangle} S_j - B_{ext}}_{\downarrow} \Big] S_i$$

$$= \big[-J \ Sum - B_{ext} \big] S_i$$

$$Sum \equiv \sum_{j=1}^{4} S_j$$

جمع روی اسپین همسایه‌های S_i

③

$$S_i^{old} \longrightarrow \boxed{S_i^{New} = -S_i^{old}}$$

$$\Delta E = \mathcal{H}^{New} - \mathcal{H}^{old}$$

$$= \mathcal{H}_i^{New} - \mathcal{H}_i^{old} = \overbrace{\big[-J \ Sum - B_{ext} \big] S_i^{New}}^{\mathcal{H}_i^{New}}$$

$$- \underbrace{\big[-J \ Sum - B_{ext} \big] S_i^{old}}_{\mathcal{H}_i^{old}}$$

$$\Delta E = \left[-J\,\mathrm{Sum} - B_{ext}\right] S_i^{New} - \left[-J\,\mathrm{Sum} - B_{ext}\right](-S_i^{New})$$

$$= 2\left[-J\,\mathrm{Sum} - B_{ext}\right] S_i^{New} = -2\left[-J\,\mathrm{Sum} - B_{ext}\right] S_i^{old}$$

$$\Delta E = \left[+2J\,\mathrm{Sum} + 2B_{ext}\right] S_i^{old}$$

How many cases. (2)

S_i^{old} → it has Two Cases ↑, ↓

2D
1. All up → Sum = +4
2. 3up - 1Down → Sum = +2
3. 2up - 2Down → Sum = 0
4. 1up - 3Down → Sum = -2
5. All Down → Sum = -4

$\Delta E(q, p)$

q → 5 حالت دارد

p → 2 حالت

۱۰ حالت داریم

$$\begin{cases} \Delta E(1,1) = \Delta E(\text{Allup}, S_i^{old} = +1) \\ \Delta E(2,1) = \Delta E(\text{3up-1Dn}, S_i^{old} = +1) \\ \Delta E(1,2) = \Delta E(\text{Allup}, S_i^{old} = -1) \end{cases}$$

$$\Delta E(q, p) = J q + B_{ext}\, p$$

$q \equiv +2\,\underset{4!}{\mathrm{Sum}}\, S_i^{old}$

$p \equiv +2\, S_i^{old}$

(4)

loop $q = -8, 4, 0, +4, +8$

loop $p = -2, +2$

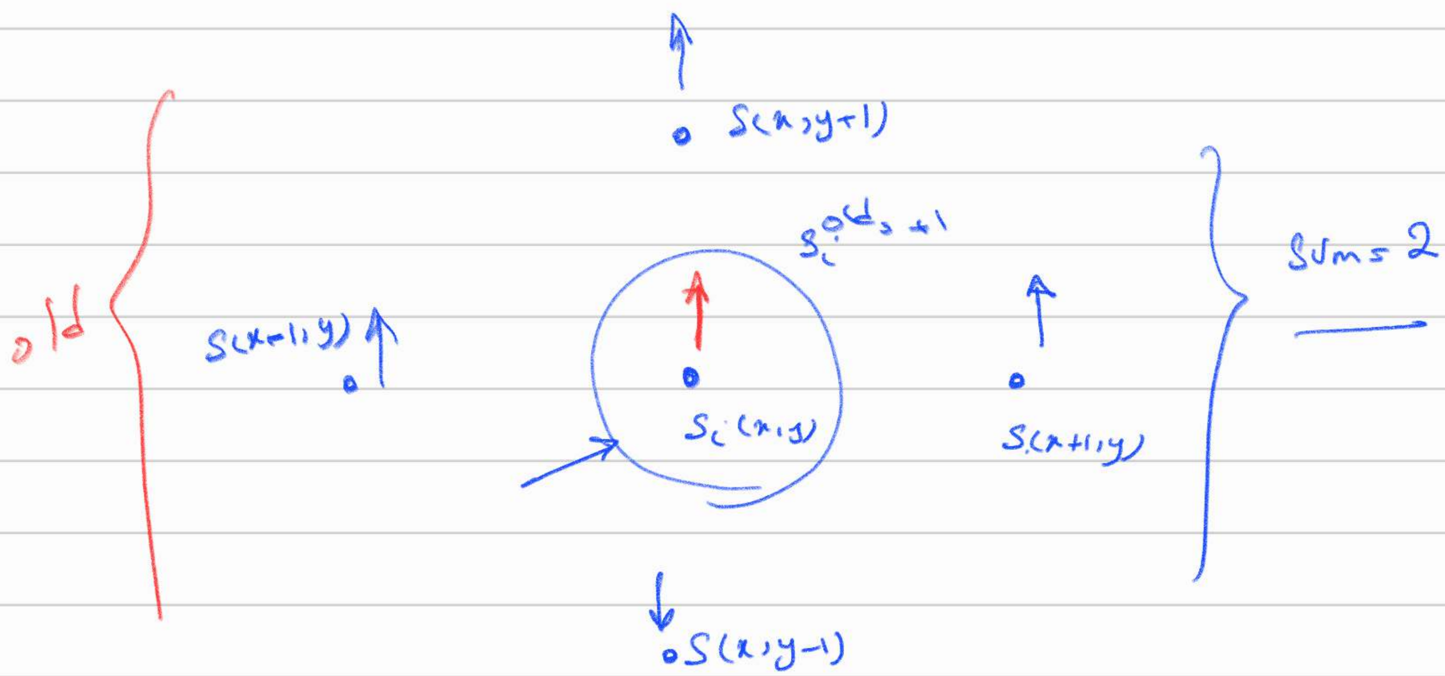
تمام حالت های ممکنی که می‌توان رخ داد.

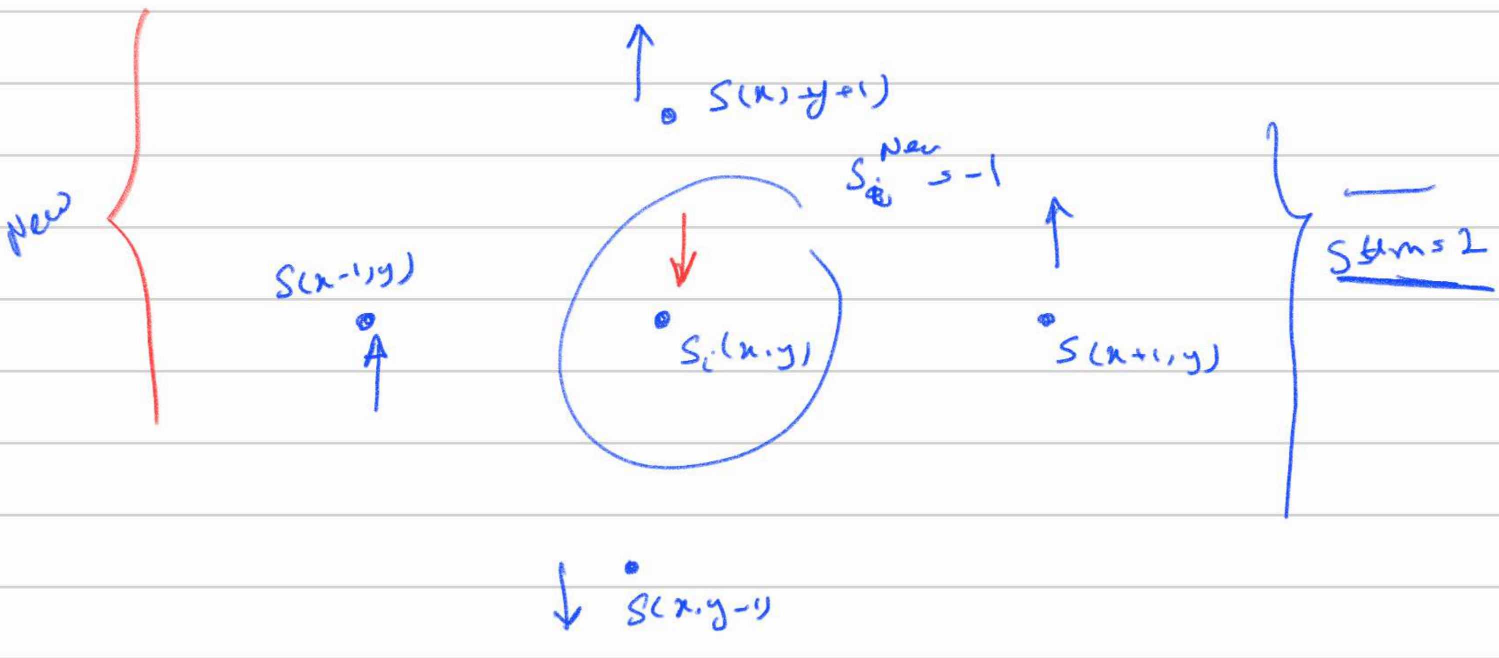
$\Delta E(q, p) = J q + B_{ext}\, p$

End loop

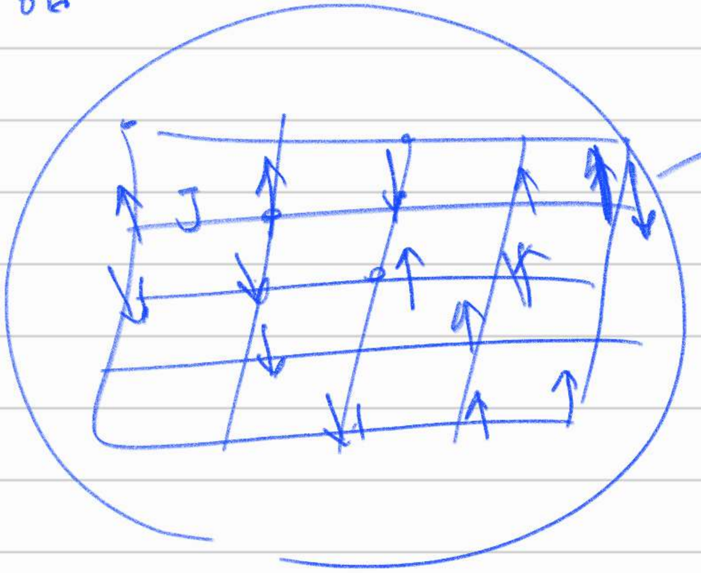
End loop

(A)

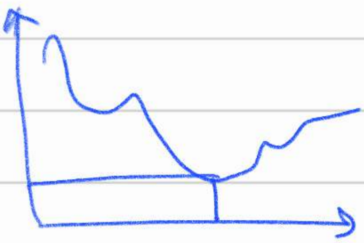




$$\{\theta\}_{old} \longrightarrow \{\theta\}_{New}$$

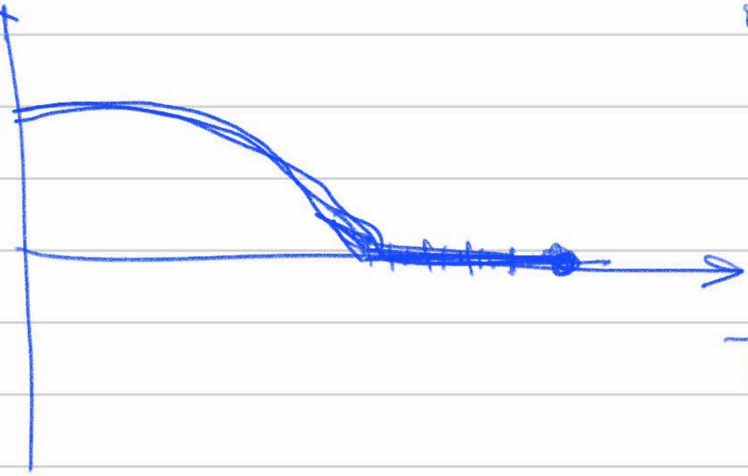


$\mathcal{H}$



$$e^{-\beta \mathcal{H}} \qquad \beta = K_B T$$

$\langle M(T) \rangle$



$$T = K_B T$$

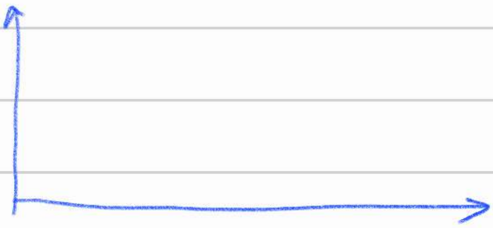
ΔT

loop $T = T_{max}$ $T_{low} = 0$

$$\int f(x)\, dx \rightarrow \int \frac{f(x)}{p(x)} p(x)\, dx = \left\langle \frac{f(x)}{p(x)} \right\rangle$$

$$= \sum_x \frac{f(x)}{p(x)}$$

$p(x)$



$$\int_{-\infty}^{+\infty} p(x)\, dx = 1$$

$$\mathcal{N}(0,1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

$f(x) = x^2$

$p(x) = N(0,1)$ $\Rightarrow$ $\displaystyle\sum_x \frac{x^2}{\frac{e^{-x^2/2}}{\sqrt{2\pi}}} =$

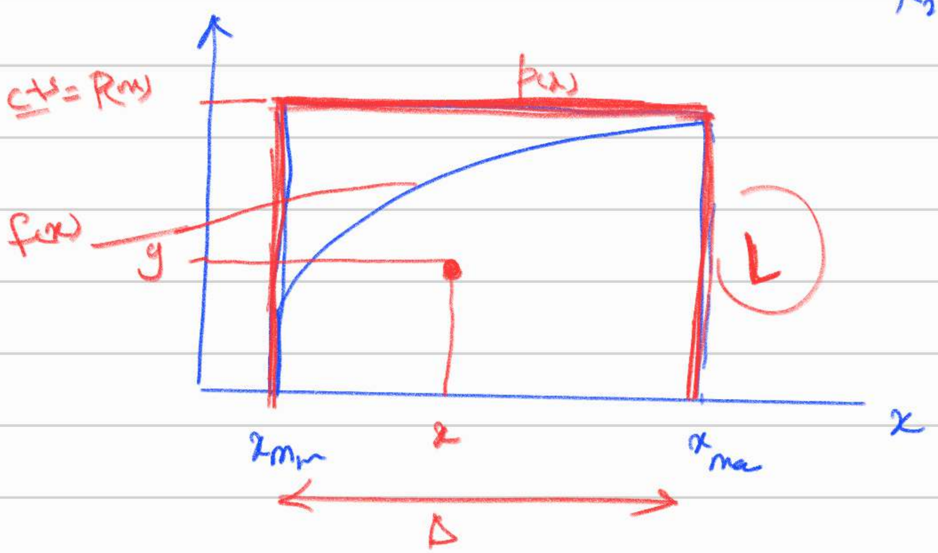
$$\int_a^b f(x)dx \simeq \left\langle \frac{f(x)}{p(x)} \right\rangle = \frac{x_1^2}{\frac{e^{-x_1^2/2}}{\sqrt{2\pi}}} + \frac{x_2^2}{\frac{e^{-x_2^2/2}}{\sqrt{2\pi}}} + \dots$$

$x \in$ Randomly Selected from Box Muller

$x \in [x_{min}, x_{max}]$ — $x = \sqrt{-2\ln(1-R_1)}\,\sin(2\pi R_2)$

$R_1 \in [0,1]$

$R_2 \in [0,1]$



$y_{Ran} \leq f(x) \rightarrow$

$$\int_{x_{min}}^{x_{max}} f(x)\,dx = ? \quad — \quad \int \frac{f(x)\,P(x)}{P(x)}\,dx$$

Probability Distribution

$$\int_{x_{min}}^{x_{max}} \overset{cts}{P(x)}\,dx = \underline{L \times \overbrace{(x_{max} - x_{min})}^{\Delta}}$$

$P(x) = \dfrac{1}{L\Delta}$ — $\int p(x)\,dx = 1$

$x \in [x_{min}, x_{max}]$ Randomly. $R \in [0,1]$

$$x = x_{min} + (x_{max} - x_{min}) R$$

$[0, 1]$

$[x_{min}, x_{max}]$

$$\int_{x_{min}}^{x_{max}} dx \, f(x) = \int_{x_{min}}^{x_{max}} \frac{f(x)}{\left(\frac{1}{L\Delta}\right)} p(x) \, dx = \left\langle \frac{f}{p} \right\rangle$$

$$= L \times \overbrace{(x_{max} - x_{min})}^{\Delta} \sum_{x \in} f(x)$$