Lecture: Critical slowing down / Advanced MC algorithms and Ising model

- consider a system at very high temperature, Ising model above T_c
  - system easily overcomes barriers, hence MC moves are easily accepted $\Rightarrow$ algorithm efficient
- if $T \to T_c$, system is less efficient at overcoming barriers
  - indeed, system starts to order, correlation length becomes larger, $\Rightarrow$ single spin-flip moves are less efficient and are accepted less

- ~~is it possible to~~

- in this case: τ increases

$$\tau \sim \xi^{z}$$

$\tau \to$ correlation time in MC passes

$\xi \to$ correlation length of model

z - dynamical critical exponent

for regular Metropolis algorithm $z \sim 2$

- cluster moves allow reduction of τ

Swendsen - Wang algorithm: first successful cluster method for Ising model

- define $\quad H_{lm} = \sum_{(i,j) \neq (l,m)} J_{ij} \sigma_i \sigma_j$

Hamiltonian without contribution from pair l,m

- construct partition functions: Z_{lm}^{same}, Z_{lm}^{diff}, Z_{lm}^{ind}

$$Z_{lm}^{same} = \sum_{\{\sigma_i\}} \exp[-\beta H_{lm}] \, \delta_{\sigma_l \sigma_m}$$

→ partition function for H_{lm} in which spins l and m are constrained to be the same

$$Z_{lm}^{diff} = \sum_{\{\sigma_i\}} \exp[-\beta H_{lm}] (1 - \delta_{\sigma_l \sigma_m})$$

→ partition function for H_{lm} in which spins l and m are constrained to be different

$$Z_{lm}^{ind} = \sum_{\{\sigma_i\}} \exp[-\beta \mathcal{H}_{lm}]$$

→ partition function for H_{lm} in which spins l and m are independent

$$Z_{lm}^{ind} = Z_{lm}^{same} + Z_{lm}^{diff}$$

partition function of the system with $H = J \sum_{\langle ij \rangle} \sigma_i \sigma_j$ can be written

$$Z = e^{-\beta J_{lm}} Z_{lm}^{same} + e^{\beta J_{lm}} Z_{lm}^{diff}$$

$$\Rightarrow Z = e^{-\beta J_{lm}} Z_{lm}^{same} + e^{\beta J_{lm}} \left(Z_{lm}^{ind} - Z_{lm}^{same} \right)$$

$$= \left(e^{-\beta J_{lm}} - e^{\beta J_{lm}} \right) Z_{lm}^{same} + e^{\beta J_{lm}} Z_{lm}^{ind}$$

for ferromagnetic coupling $J_{lm} < 0$

$$\Rightarrow \left(e^{-\beta J_{lm}} - e^{\beta J_{lm}} \right) > 0$$

moreover in this case

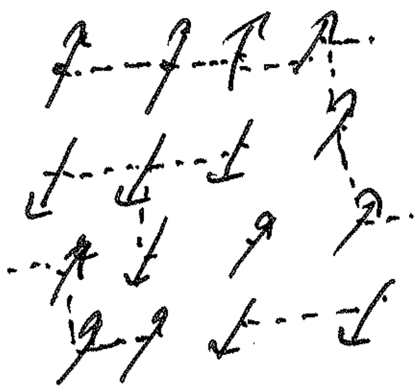
$$Z = A Z_{lm}^{same} + B Z_{lm}^{ind}$$

$\Rightarrow$ partition function consists of a term ~~accord~~ in which the spins are the same (probability $A/(A+B)$) and one in which the spins are independent (probability $B/(A+B)$)

- cluster MC method can be constructed as follows:

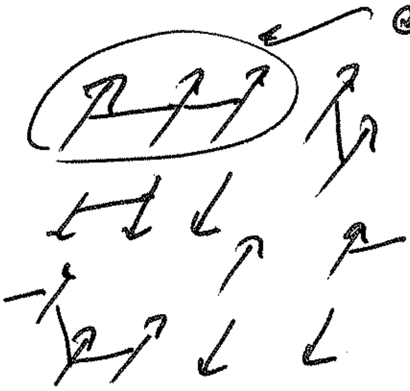
- consider ~~one~~ bonds which connect parallel spins
- loop through all such bonds, and keep each such bond with probability $\frac{A}{A+B}$
- the bonds which have been kept will form clusters
- flip each cluster with 50% probability

⇒ example:
configuration before cluster move



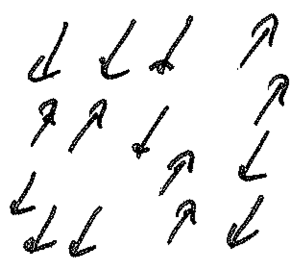
⇒ all parallel spin bonds considered

- loop through and keep each bond w/ probability $A/(A+B)$



example of a cluster (this is one possibility)

- flip each cluster w/ 50% probability



- after start over again

- this algorithm reduces τ to ca. 0.5
- for antiferromagnetic case ($J_{lm} > 0$)

$$Z = \cancel{Z^{diff}_{lm}} + (e^{\beta J_{lm}} - e^{-\beta J_{lm}}) Z^{diff}_{lm} + e^{\beta J_{lm}} Z^{ind}_{lm}$$

- cluster bonds connect configurations which are bonded with bonds connecting anti-parallel spins
- one can also show that the detailed balance condition is satisfied

$$Z = (e^{-\beta J_{lm}} - e^{\beta J_{lm}}) Z^{same}_{lm} + e^{\beta J_{lm}} Z^{ind}_{lm}$$

$$\cancel{= e^{\beta J_{lm}}(e^{-2\beta J_{lm}} - 1)}$$

$$= e^{-\beta J_{lm}} \left[(1 - e^{2\beta J_{lm}}) Z^{same}_{lm} + e^{2\beta J_{lm}} Z^{ind}_{lm} \right]$$

- for simplicity assume $J_{lm} = J$ and consider a 1D system

↗ ↗ ↙ ↙ ↙ ↗ ↗ ↗ ↙

suppose bonds deleted are

(⇒ 2 bonds deleted)

↗ ↗ ↙ ↙ ↙ ↗ ↗ ↗ ↙

flip (50%)

↗ ↗ ↙ ↙ ↗ ↙ ↙ ↗ ↙

consider backward route → in this case no bonds

$\nearrow\!-\!\nearrow \swarrow \nearrow\!-\!\nearrow \swarrow\!-\!\swarrow \nearrow \swarrow$ are deleted

flip

$\nearrow\nearrow\swarrow\swarrow\swarrow \nearrow\nearrow\nearrow\swarrow$ → original configuration

probability of forward route: $e^{2\beta J\cdot 2}$

two deleted bonds

probability of backward route: 1

relative probability $e^{4\beta J}$

- the relative probability when we compare the two configurations

$\nearrow\nearrow \swarrow\swarrow\swarrow \nearrow\nearrow\nearrow\swarrow \rightarrow e^{\beta J(5-4)} = e^{\beta J}$

$\nearrow\nearrow\swarrow\nearrow\nearrow \swarrow\swarrow\nearrow\swarrow \rightarrow e^{\beta J(3-6)} = e^{-3\beta J}$

relative probability: $\dfrac{e^{\beta J}}{e^{-3\beta J}} = e^{4\beta J}$

---

general proof

- suppose n_1 bonds eliminated in forward step, and n_2 bonds are eliminated in backward step

$\Rightarrow$ relative probability: $e^{2\beta J(n_1-n_2)}$

~~→ [illegible]~~

→ same as relative probability of configurations

MC algorithms for Ising model are not limited to nearest neighbor coupling and zero field, like the exact solution

⇓

can also solve models with randomly assigned bonds (random Ising model) which is an important model for spin glasses