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Discussion of Simulations of MH or Glauber algos for the Ising model.

First Recap from course:

- $$\mathcal{H}(\underline{S}) = -\sum_{(i,j)\in E} \frac{J}{N} S_i S_j - h\sum_{i\in V} S_i$$

$J > 0$: ferromagnetic model, $h \in \mathbb{R}$

Here $G = (V, E)$ is the complete graph and we have $O(N^2)$ edge hence the $\frac{J}{N}$ scaling to balance both terms in $\mathcal{H}$.

- Gibbs distr
$$\pi(\underline{S}) = \frac{e^{-\beta \mathcal{H}(\underline{S})}}{Z}, \quad \underbrace{\beta}_{\text{inverse temperature}} > 0 \qquad \frac{1}{T}.$$

$$Z = \sum_{\underline{S}\in\{-1,+1\}^N} e^{-\beta \mathcal{H}(\underline{S})}$$

- MH or Glauber ; $t = 0, 1, 2, 3 \ldots$

Start with $\underline{S}(0)$. Select $v \in V$ at random. Flip $S_v \to S_v^{New} = -S_v$ with probability :

$\underline{MH} \to \min(1, e^{-\beta\Delta})$; $\Delta = \mathcal{H}(\underline{S}^{New}) - \mathcal{H}(\underline{S})$

$\underline{\text{Glauber}}$ $\underbrace{\frac{1}{2}\left(1 - S_v \tanh h_v^{loc}\right)}$; $h_v^{loc} = \frac{J}{N}\sum_{w\neq v} \sigma_w$

(tendency to make $S_v^{New} \cdot h_v^{loc} > 0$ to minimize $\mathcal{H}$.)

• Now we want to look at behavior of "magnetization" when we run the MCMC

$$m(t) \equiv \frac{1}{N} \sum_{v \in V} S_v(t) \qquad |V| = N.$$

<u>What do we expect ?</u>

For N finite the chain is ergodic so you expect that

$$\lim_{T \to +\infty} \lim_{t \to +\infty} \frac{1}{T} \int_t^{t+T} d\tau \, m(\tau) = m^{\text{stationary}}$$

eliminate transient behavior.

average over time (equiv to average over many runs of the chain).

where $m^{\text{stationary}} = \mathbb{E}_{\pi}\left[\frac{1}{N} \sum_{i=1}^{N} S_i \right] = \left\langle \frac{1}{N} \sum_{i=1}^{N} S_i \right\rangle$

expectation w.r.t to Gibbs (stationary limiting distr).

($\langle - \rangle$ is just another notation).

When $h = 0$ $m^{\text{stat}} = 0$. So we expect for finite N this time average should be zero. This is true but DOES IT GIVE THE RIGHT INTUITION?

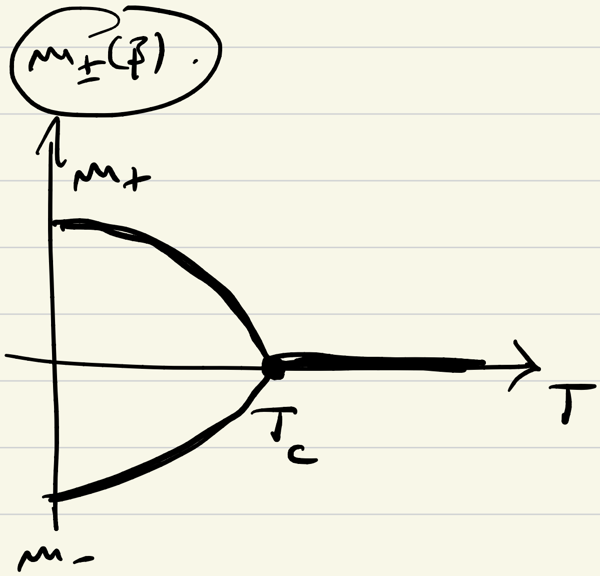
- There is much more hidden behind this. It is worth looking at more detailed view of MCMC chain.

Lets go back to equilibrium situation (or study of the Gibbs measure).

define $\underbrace{m(\beta, h)}_{m^{\text{stationary}}} = \frac{1}{N} \left\langle \sum_{i=1}^{N} s_i \right\rangle (\beta, h)$.

and $m_{\pm}(\beta) = \lim_{h \to 0_{\pm}} m(\beta, h)$.

One can show (for Ising ferro on complete graph one can do the exact computation)

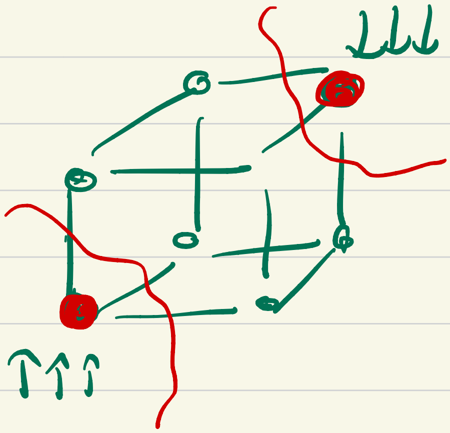


"Picture of typical configurations" of Measure:

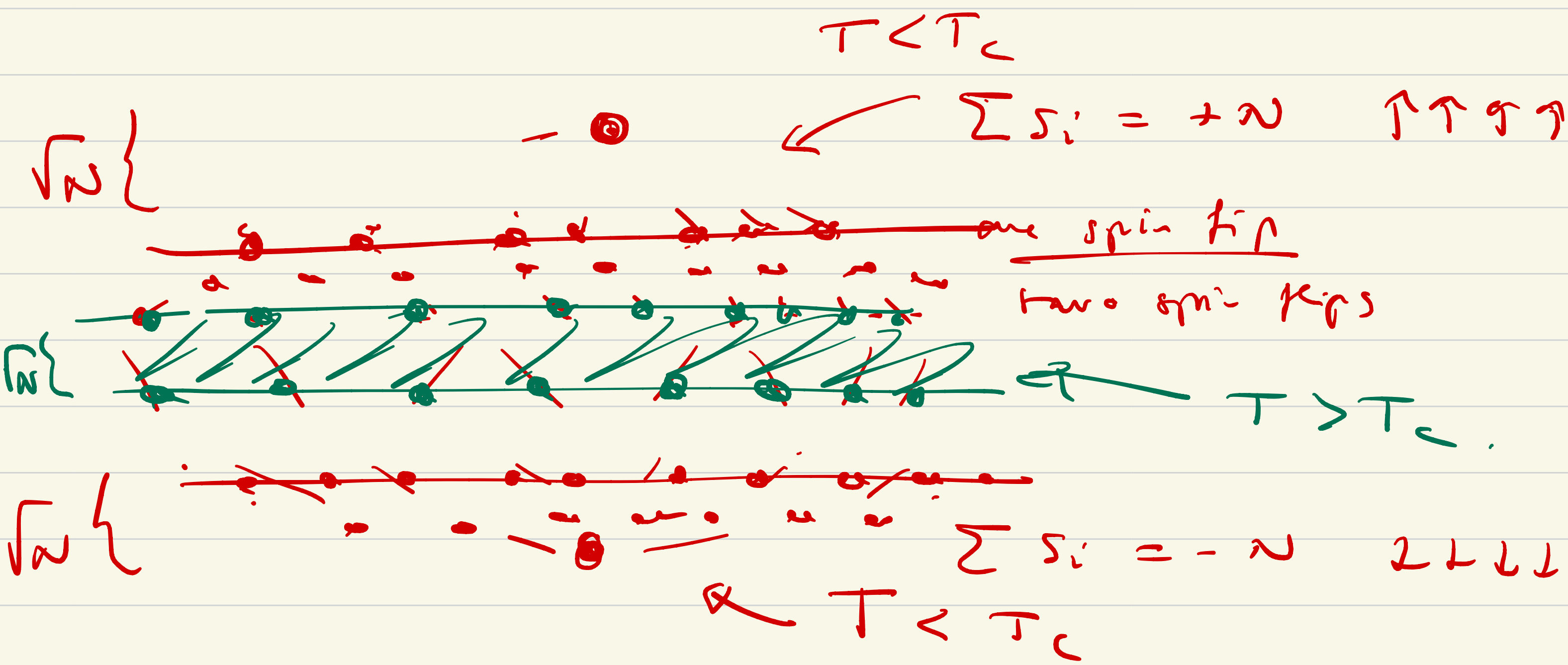
- $T > T_c$ Meas supported on typ conf s.t $\sum_{i=1}^{N} s_i \simeq 0$ up to $\sqrt{N}$ fluctuations

- $T < T_c$ Meas supported on typ conf s.t $\sum_{i=1}^{N} s_i = \pm N m_+$ up to $\sqrt{N}$ fluctuations.

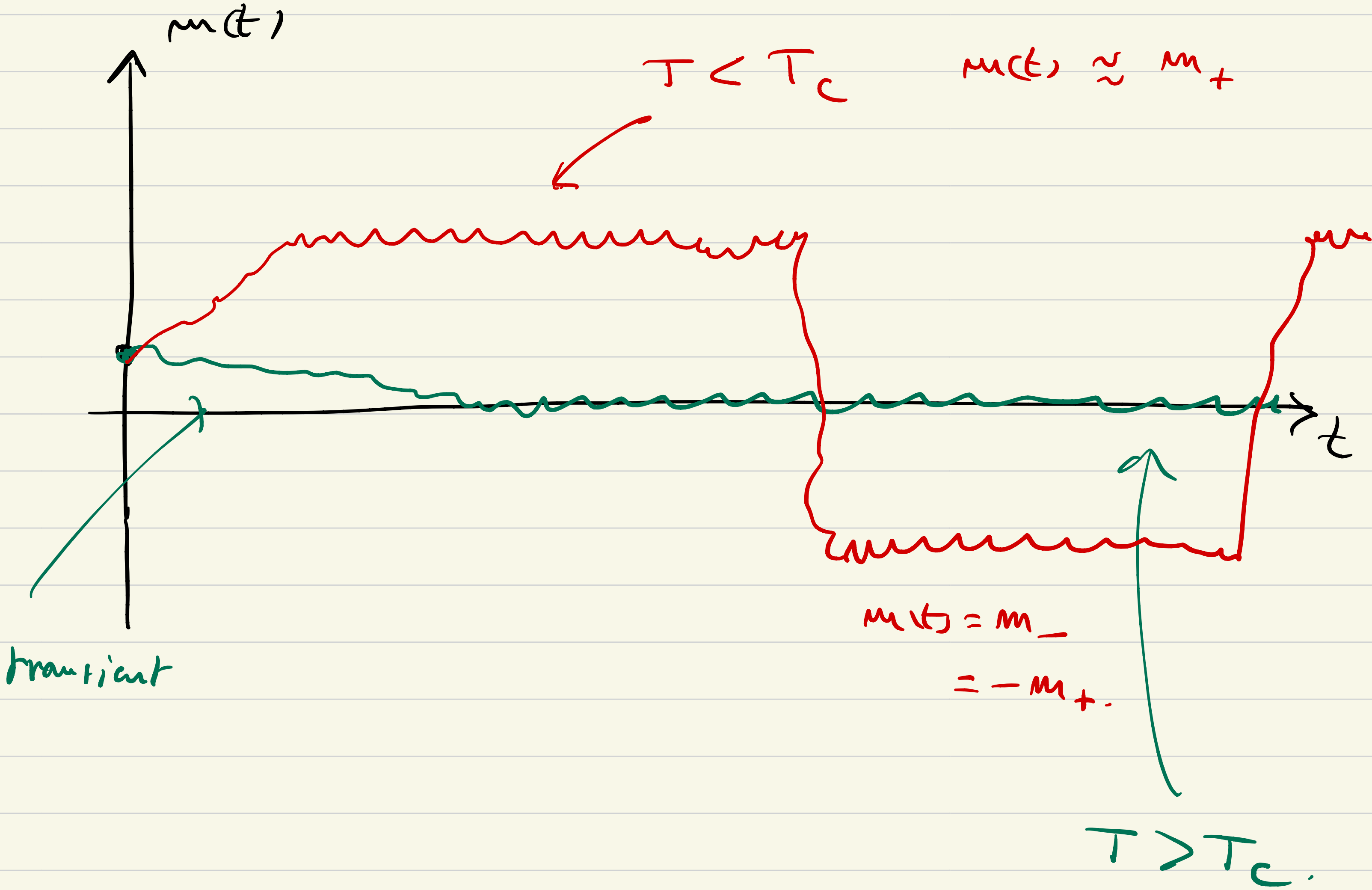
"Hamming cube" or "Hasse diagram"



- $T < T_c$ Measure splits on "two clusters"
- $T > T_c$ Measure supported on whole cube.



Trajectories of MCMC:



$$\begin{cases} T > T_c & \text{mixing time } \quad O(N \log N) \\ T < T_c & \text{mixing time enormous } \sim e^N \end{cases}$$

Consistent with $\displaystyle \lim_{T \to +\infty} \lim_{t \to +\infty} \frac{1}{T} \int_t^{t+T} ds\, m(s) = 0$

and ergodic Thm. BUT the ergodic Thm does not tell the whole detailed story here ....