MONTE-CARLO SIMULATIONS

① Pathria - Beale.
② ArXiv 1101.3281

Our objective here is to simulate the 2D Ising model on a lattice and thereby compute the 'critical coefficients'.

SAMPLING:

At a given temperature, various microscopic states occur with a probability distribution $P_e(\beta) = e^{-\beta E}$ where E is the total energy of the entire 'single' configuration. (e ← equilibrium)

An average of any quantity Q is provided by

$$\langle Q \rangle = \sum_{\{s_i\}} Q\, e^{-\beta E}$$

For Ising (nearest neighbour)

$$E = -J \sum_{\langle ij \rangle}' s_i s_j$$

Thus this average can be found after randomly choosing micro states $\alpha = \{s_i\}$ and thereafter performing average, over a collection of samples $\{\alpha\}$ weighted by $e^{-\beta E}$.

The idea in MC is: instead of choosing configs randomly and then weigh them with $P_e(\beta)$, choose configurations with a probability $e^{-\beta E}$ and weigh them evenly.

Choose a sample → keep it or throw it away with probability $P_e(\beta)$.
(Decision is made using a (pseudo) random no. generator and comparing it with $P_e(\beta)$ [More later]).

Principle of Detailed Balance

Consider dynamics - time evolution.

→ System prepared in a given microstate and allowed Hamiltonian time evolution, at some temperature (β).

→ Ergodicity ensures system moves over various microstates, and equilibrates at late times.

Let $P_{eq}(\beta; \alpha) :=$ Probability system in microstate α when in equilibrium at temperature β.

→ Out-of-equilibrium dynamics → Allow discreet time steps.

Assume Markovian process: Each time-step only determined by config in previous time step.

Allow the system to evolve according to discrete stochastic rate eqn.

probability during out-of-equilibrium dynamics.

$$P(\beta; \alpha, t = t+1) = \sum_{\alpha'} P(\beta; \alpha', t)\, W(\alpha' \to \alpha).$$

→ A random walk in the space of configurations.

where $W(\alpha' \to \alpha)$ is the stationary transition probability from microstat α' to α.

To ensure Ergodicity: $\lim_{t \to \infty} P(\beta; \alpha, t) = P_{eq}(\alpha)$

(1) We need a balance condition: [take $t \to \infty$ limit of rate eqn.]

$$\sum_{\alpha'} P_{eq}(\beta; \alpha') W(\alpha' \to \alpha) = P_{eq}(\alpha) \sum_{\alpha'} W(\alpha \to \alpha')$$

If this is 1 eq. (1) is satisfied

probability of going from a given state to any other state α'.

(2) Every microstate should be reachable starting from another in finite time.

A special way to satisfy the balance condition is **detailed balance**

Time reversability

$$P_{eq}(\beta;\alpha)\, W(\alpha\to\alpha') = P_{eq}(\beta;\alpha')\, W(\alpha'\to\alpha).$$

In general W has 2 factors
$W = W_{select}\, W_{accept}$
One spin is selected at a time with equal probability.

We can write

$$W(\alpha\to\alpha') = e^{(-\beta\Delta E)}\, W(\alpha'\to\alpha).$$

⇒ Sample states by performing a stochastic random walk among equilibrium microstates.

$W(\alpha\to\alpha') = \min(1, e^{-\beta\Delta E})$

Metropolis Algorithm : A solution to detailed balance condition.

$W(\alpha\to\alpha') = 1$ if $\Delta E = E_\alpha - E_{\alpha'} \leq 0$.

$W(\alpha\to\alpha') = \exp(-\beta\Delta E)$ if $\Delta E > 0$.

Implementation of steps in a Computer (keep 2D Ising in mind).

Hamiltonian : $H = -J \sum_{\langle ij\rangle} S_i S_j$ [40×40 lattice to start with].

can be explicitly evaluated if we know all the spins.

① Start with $\alpha = \alpha_0$ at $t=0$ for a given β : α_0 can be all up for any β.

② Ensure periodic boundary conditions.

③ Flip spin no. 1 (S_1) [going from $\alpha\to\alpha'$] → evaluate $\exp(-\beta\Delta E)$.

Keep new config with probability

$W(\alpha\to\alpha') = 1$ if $\Delta E = E_\alpha - E_{\alpha'} \leq 0$.

$W(\alpha\to\alpha') = \exp(-\beta\Delta E)$ if $\Delta E > 0$.

↑ Determine by selecting a random no. between 0-1, if $r < \exp(-\beta\Delta E)$ then accept.

1 MC step.

④ Repeat 1 MC step for spins located at all sites → 1 MC cycle.

1 MC cycle = 1 'time' step [Monte-Carlo time] (t_m).

⑤ Repeat MC cycle for large $t_m^{(eq)}$ (eg. $t_m \sim 10^3$-10^4 - more near PT).
This is step for equilibriation.

⑥ Start collecting sample configurations after $t_m^{(eq)}$.
Store / compute physical quantity and throwaway

→ Wait for $t_m^{(a)}$ in between collection of sample to remove auto-correlations between samples. [Collect independent samples].
You may consider auto correlations in Energy / magnetization. [Q]

$$\text{Auto correlation in } Q = A_Q(t_m) = \frac{\langle Q(i+t_m)\,Q(i)\rangle - \langle Q\rangle}{\langle Q^2\rangle - \langle Q\rangle^2}$$

averages are over reference times.

In general, $A_Q(t_m) \sim e^{-t/\tau_Q}$

$\tau_Q^{(m)}$:= Auto corelation time.

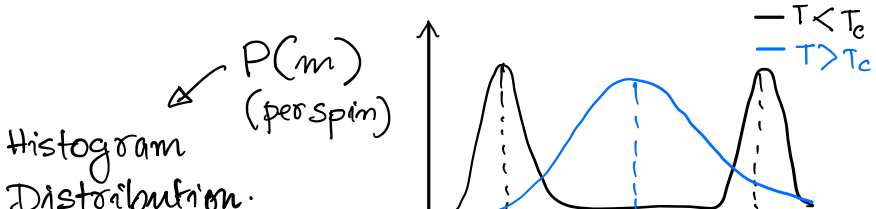
Waiting time between sample collection $\tau_Q^{(m)} = t_m^{(a)}$ ($\sim 10^2$)

Equilibriation time $t_m^{(eq)}$ a few orders of magnitude more than auto correlation time.

⑦ Collect large (N) no. of samples ($N \approx 10K$). for a set of values of Temperature
(to ensure sample average = actual average).

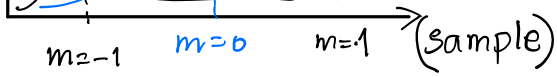
Conside T at an interval of 0.2 for a reasonable range which includes T_c

⑧ Measure physical quantities from sample after averaging (for every T).
eg: Probability distribution of magnetization below & above T_c



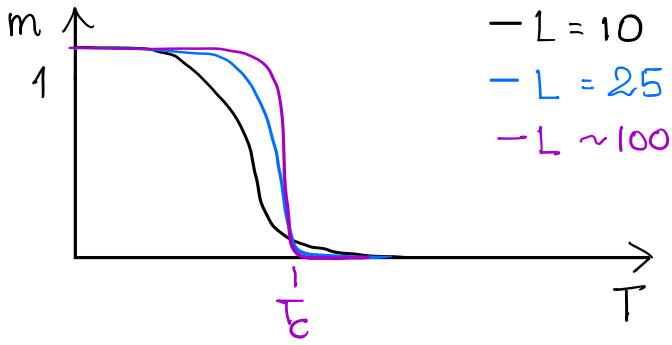
Ex. plot probability distribution of Energy.

$$m = \frac{1}{N}\sum_i S_i$$

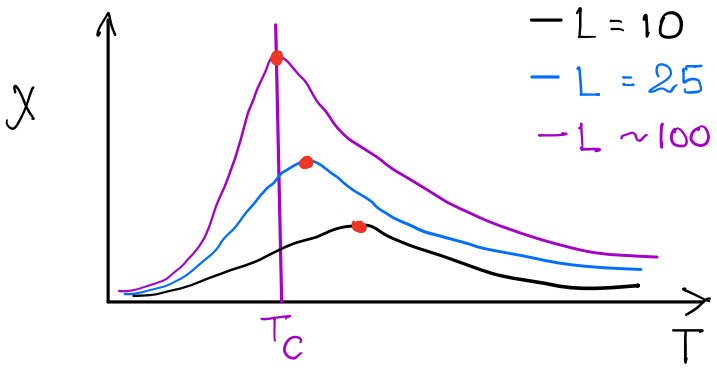


$s_i = \{\pm 1\}$.

(9) Measure T_c by FINITE SIZE SCALING:



As we increase L (no. of lattice points) transition becomes sharper.



$m=\pm 1$ are treated uniformly

$$\chi = \left.\frac{\partial m}{\partial h}\right|_{h\to 0} = \frac{N}{T}\left(\langle m^2\rangle - \langle |m| \rangle^2\right)$$

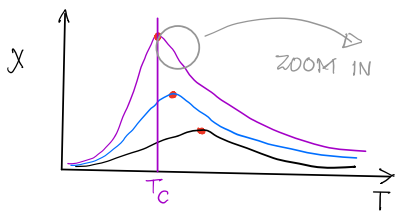
Maxima shifts towards T_c value as we increase L.

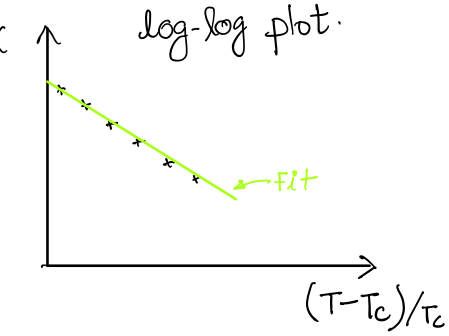
(10) After ploting m, χ, C for the system

(i) estimate the scaling exponents α, β, γ.

(ii) Also estimate the universal ratios χ_+/χ_-, C_+/C_-.

For computing scaling coefficients (for eg. χ), you may use the following method:





$$\begin{cases} \chi = \chi_+ \left(\frac{T-T_c}{T_c}\right)^{-\gamma} \\ \ln\chi = -\gamma \ln\left(\frac{T-T_c}{T_c}\right) + \ln\chi_+ \end{cases}$$

slope, intercept

Similarly, find the exponent below T_c.

As we increase T_c we have a better fit to straight line near T_c. (in Log-log plot).

(11) Two point function near T_c. :

$$G(r_j) = \frac{1}{L} \sum_{i=1}^{L} \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle$$

where $\langle\ \rangle$ denotes average over all sample configs at a given temperature T.

One of the points in 2pt func. is averaged over all lattice points.

For large r_j display a log-log plot of $G(r_j)$ to obtain scaling coefficient η.