Appendix B: Metropolis Monte Carlo Algorithm (Practical Steps) [Optional]

How to study, say, Ising Model by simulations?

Recall: Canonical Ensemble (T,V,N)

- $e^{-E_i/kT} \propto$ Prob. of having the system in a state of energy E_i
- But # states (N-particle system) of energy E_i depends on E_i

Select members of a collection (ensemble) properly $\Rightarrow$ Importance Sampling

Is there a practical way to do that?

Here is a standard method (within the context of Ising Model)

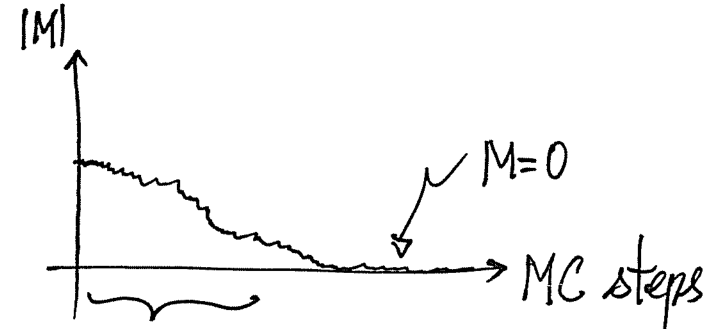
Ising Model : Monte Carlo Simulation

- 2D square lattice, assign +1, −1 randomly (initialization)
- In a time step,
  - randomly pick a spin and attempt a spin flip (up to down/down to up)
  - Evaluate change in energy due to attempt spin flip ΔE
  - If $\Delta E < 0$, accept the flip. Start a new step.
  - If $\Delta E > 0$, accept the flip with a probability $e^{-\Delta E/kT}$, otherwise reject the flip. Start a new step.
- Monte Carlo Step: When each spin went through one attempt
- Repeat procedure for many MC steps
- Record data, e.g. energy E, magnetization m, as MC steps proceed

Done!

[There are ready-to-use programs on the web and in textbooks on computational physics]

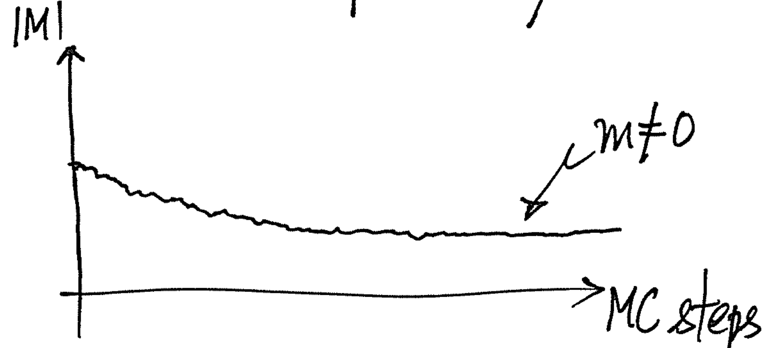
Given T: $(T>T_c)$



transient (depends on your initial conditions)

[May discard initial MC steps before taking average]

$(T<T_c)$



And record E as MC steps.

$$(\Delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2 = kT^2 C_V$$

$$\Rightarrow C_V = \frac{1}{kT^2} \underbrace{(\Delta E)^2}$$

can be obtained by simulations

way to get heat capacity

The point is :

- There are practical (and clever) ways to sample the different states of an interacting system according to the Canonical Ensemble.
- Metropolis algorithm is a way to do that.

Refs :

H. Gould and J. Tobochnik, "An Introduction to Computer Simulation Methods : Applications to Physical Systems"