

Monte Carlo simulations (Canonical ensemble)

(brief description in Kardar;

detailed textbooks: Newman & Barkema
Binder & Heermann)

$$P[\alpha] = \frac{1}{Z} e^{-\beta E[\alpha]}$$

↑
model configurations (e.g., spin configuration

$$d = \{S_i\}_{i=1, \dots, L} \quad \text{for Ising spin, } \alpha = 1, 2, \dots, 2^L$$

$$\langle O \rangle = \sum_{\alpha} O(\alpha) P(\alpha)$$

usually, there are prohibitively many configs. to do the sum directly; can try "Monte Carlo integration"

Bad approach: random sampling — generate completely random configs. $\alpha_k, k=1 \dots M$, and approximate

$$\langle O \rangle \approx \frac{\sum_k O(\alpha_k) e^{-\beta E[\alpha_k]}}{\sum_k e^{-\beta E[\alpha_k]}}$$

— very poor approach because random configs will typically have very small statistical weight (wasted effort)

Good approach: importance sampling — generate

configs $\alpha_k, k=1 \dots M$, with probability proportional to $P[\alpha]$

$$\langle O \rangle \approx \frac{1}{M} \sum_{k=1}^M O[\alpha_k]$$

— good because the sampling proceeds only over configs with large stat. weight (important configs.)

Generating importance sampling

Consider stochastic process (Markov process)

$\alpha \rightarrow$ generate β with probability $\Pi_{\alpha \rightarrow \beta}$ } irrespective of the history, i.e. no memory

$\Pi_{\alpha\beta} = \Pi_{\alpha \rightarrow \beta}$ - matrix of transition probabilities, satisfying

$$\begin{aligned} \Pi_{\alpha\beta} &\geq 0 \quad (\text{probabilities cannot be negative}) \\ \sum_{\beta} \Pi_{\alpha\beta} &= 1 \quad (\text{sum of all probabilities is 1}) \end{aligned}$$

Suppose at $t=0$ we start in config α with probability $p_{\alpha}(t=0)$ (e.g., generating α at random: $p_{\alpha}(t=0) = \frac{1}{\text{total \# of configs.}}$)

$$p_{\alpha}(t=1) = \sum_{\beta} p_{\beta}(t=0) \Pi_{\beta \rightarrow \alpha} = (\hat{\Pi}^T \vec{p}(t=0))_{\alpha}$$

$$\vec{p}(t) = \hat{\Pi}^T \vec{p}(t-1) = \dots = \underbrace{(\hat{\Pi}^T)^t}_{t \text{ times}} \vec{p}(0)$$

Claim: the largest eigenvalue of $\hat{\Pi}^T$ is 1; the corresponding eigenvector $\vec{p}^*$ is non-negative and is called stationary probability distribution for this Markov process:

$$\hat{\Pi}^T \vec{p}^* = \vec{p}^*$$

Perron-Frobenius theorem $\rightarrow$

Proof: consider $\hat{\Pi}$ which has only non-negative entries. The eigenstate with the largest eigenvalue must have all components non-negative. On the other hand, $\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$ has non-negative components and is eigenstate with eigenvalue 1: $\hat{\Pi} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \alpha \begin{pmatrix} \sum_{\beta} \Pi_{\alpha\beta} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$

$\Rightarrow$ the largest eigenvalue of $\hat{\Pi}$ is 1; $\Rightarrow$ the largest eigenvalue of $\hat{\Pi}^T$ is 1 $\blacktriangle$ eigvals of $\hat{\Pi}$ & $\hat{\Pi}^T$ coincide

After many applications of $\hat{\Pi}^T$, obtain the stationary distribution irrespective of the original $\vec{p}(t=0)$.

$$\vec{p}(t \rightarrow \infty) \approx \vec{p}^*$$

Want to find Markov process such that the stationary distribution is

$$p_\alpha^* = \frac{1}{Z} e^{-\beta E[\alpha]} = P^{\text{desired}}[\alpha]$$

- can achieve this, e.g., if $\Pi_{\alpha \rightarrow \beta}$ satisfies detailed balance

$$p_\alpha^{\text{desired}} \Pi_{\alpha \rightarrow \beta} = p_\beta^{\text{desired}} \Pi_{\beta \rightarrow \alpha}$$

Indeed, in this case

$$\sum_\beta p_\beta^{\text{desired}} \Pi_{\beta \rightarrow \alpha} = \sum_\beta p_\alpha^{\text{desired}} \Pi_{\alpha \rightarrow \beta} = p_\alpha^{\text{desired}}$$

and $\vec{p}^{\text{desired}}$ is an eigenstate of $\hat{\Pi}^T$ with eigenvalue 1, i.e., the stationary distribution.

Stat. mech. simulations:

$$\frac{\Pi_{\alpha \rightarrow \beta}}{\Pi_{\beta \rightarrow \alpha}} = e^{-\beta(E_\beta - E_\alpha)} = e^{-(E_\beta - E_\alpha)/kT}$$

↑
inverse temperature

Metropolis's algorithm (ignoring "configurational factors" affecting attempt frequencies)

$\alpha \rightarrow$ generate β in some prescribed way independent of energies (e.g. pick random spin and flip it);

accept β with probability $\min\{1, e^{-\beta(E_\beta - E_\alpha)}\}$
(otherwise keep α)

$$\pi_{\alpha \rightarrow \beta} = \min \{1, e^{-\beta(E_{\beta} - E_{\alpha})}\} = \begin{cases} 1, & \text{if } E_{\beta} < E_{\alpha} \\ e^{-\beta(E_{\beta} - E_{\alpha})}, & \text{if } E_{\beta} > E_{\alpha} \end{cases}$$

$$\frac{\pi_{\alpha \rightarrow \beta}}{\pi_{\beta \rightarrow \alpha}} = e^{-\beta(E_{\beta} - E_{\alpha})} \quad - \text{satisfies detailed balance}$$

Remark:

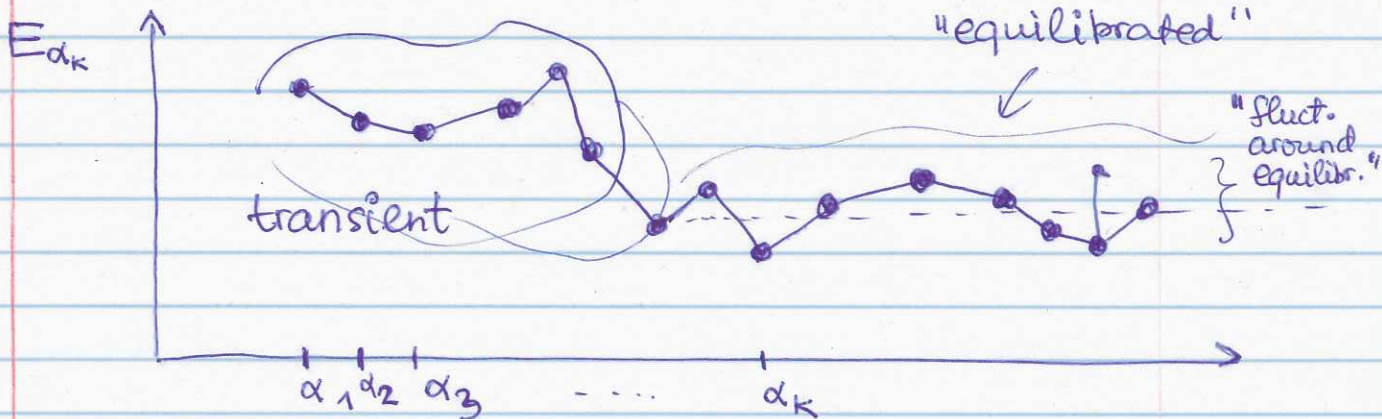
* In the above, it is implicitly assumed that the generation frequency ^{satisfies:} $q_{\alpha \rightarrow \beta} = q_{\beta \rightarrow \alpha}$ (generation before Metropolis' ~~xxx~~ acceptance test).

This is the case for simple Monte Carlo like "select spin at random and flip it", but can be violated for more complicated processes, in which case one needs to modify the Metropolis' acceptance test to account for $q_{\alpha \beta} \neq q_{\beta \alpha}$.

Implementation (general)

Illustrate
with Ising
model
in parallel

- Start with some state α ("old state")
- Select some new state β (random)
- Accept β with probability $\min\{1, e^{-(E_\beta - E_\alpha)/k_B T}\} =$
$$= \begin{cases} 1, & \text{if } E_\beta < E_\alpha \\ e^{-(E_\beta - E_\alpha)/k_B T}, & \text{if } E_\beta > E_\alpha \end{cases}$$
- If accepted, take β as "old state", i.e. set $\alpha = \beta$
If not accepted, keep α as "old state"
- Repeat
- Exclude initial transients from averaging



Remarks * computer memory needed is $\sim$ size of the lattice (L)

* computer time $\sim M$ - number of simulated states

* random number generator is needed for

- producing new state
- deciding whether to accept it or not

~~* There exists an efficient algorithm for Grand Canonical Ensemble~~

Simple Monte Carlo for Ising model

Example: Ising model

Monte Carlo step: from a given configuration

$$\alpha = \{\epsilon_1, \epsilon_2, \dots, \epsilon_{i_0}, \dots, \epsilon_L\}$$

$$\beta = \{\epsilon_1, \epsilon_2, \dots, -\epsilon_{i_0}, \dots, \epsilon_L\}$$

$$\Delta E = E_\beta - E_\alpha$$

$$= 2 \sum_{j \in i_0} J_{ij} \epsilon_i \epsilon_j$$

$$+ 2 h_{i_0} \epsilon_{i_0}$$

$\alpha = \{\epsilon_i\}$, select a spin at random, say i_0 , and attempt to flip it $\epsilon_{i_0} \rightarrow -\epsilon_{i_0}$.

Calculate energy change ΔE it would produce and accept with probability

$$\min\{1, e^{-\beta \Delta E}\}$$

|| satisfies detailed balance

Measurement

$$\langle O \rangle \approx \frac{1}{T} \sum_{t=\tau+1}^{\tau+T} O[\{\epsilon_i(t)\}]$$

(discarding initial τ steps as equilibration).

All stat mech models in this course can be studied using simple Monte Carlo

Logistics: * one measures thermodynamic quantities like energy, specific heat, and can monitor these to detect transitions

* one measures order parameter(s) (if available) and can detect phases this way (magnetization; stiffness, etc.)

* for detailed studies of critical properties, one uses finite size scaling techniques.

$$U = \langle E \rangle \approx \frac{1}{M} \sum_{k=1}^M E[\alpha_k] \quad \text{-- average energy}$$

$$C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \quad \text{-- specific heat (need to measure } \langle E^2 \rangle \text{ \& } \langle E \rangle)$$

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T} \quad \text{-- susceptibility (need to measure } \langle M^2 \rangle \text{ \& } \langle M \rangle)$$