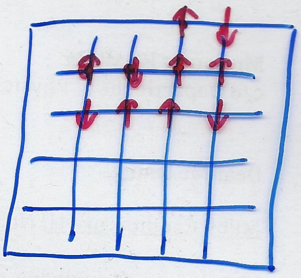
Metropolis algorithm (1953).

$$H = J \sum_{\langle ij \rangle} S_i S_j \,, \quad S = \pm \frac{1}{2}$$



each configuration has energy E_i

* many degrees of freedom.

Our task $\langle y \rangle = \dfrac{\sum_i y_i e^{-\beta E_i}}{\sum_j e^{-\beta E_j}}$ $\equiv Z$.

* how to do it numerically ?

(1). brute force — impossible to do for large systems

(2). MC $\langle y \rangle = \sum_i y_i P_i$, where $P_i = \dfrac{e^{-\beta E_i}}{Z}$.

We want to generate a sequence of state y_i with probability P_i, y_1, y_2, y_3 (not equal probability)

then $\langle y \rangle = \dfrac{y_1 + y_2 + \cdots + y_N}{N}$

* We use $x_1, x_2, \cdots$, to label states, after a small change of system parameter, we have

$$X_t = X_n + \delta$$

decision to make, whether to accept X_t as part of our distribution or sequence.

define $r = \dfrac{P(X_t)}{P(X_n)}$, $P(X_t) \propto e^{-\beta E(X_t)}$.

if $r \geq 1$, X_t is accepted, and $X_{n+1} = X_t$

if $r < 1$, $X_{n+1} = X_t$ with probability r.

This is realized by a random number, $x \in [0, 1]$.

if $x > r$, reject. if $x \leq r$ accept.

* This way, we can generate $P_i \propto \dfrac{e^{-\beta E_i}}{Z}$.

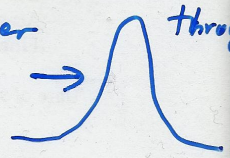
Physically, $r > 1$ means $P(X_t) > P(X_n)$, $P \propto e^{-\beta E}$

or $E_t < E_n$, the system is moving to a lower energy, accept.

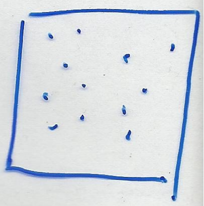
$r < 1$, means $E_t > E_n$ a barrier

tunneling probability $\sim P_i = e^{-\beta(E_t - E_n)} \rightarrow$

tunnel through



Proof. Suppose we have many states $X_1, X_2, \cdots, X_n$ in configuration space. We can talk about density of points or density of states $N(X)$ around X.



In equilibrium, we have detailed balance condition

$$N(X)\, T(X \rightarrow Y) = N(Y)\, T(Y \rightarrow X)$$

starting from X, and Y is a trial state.

a). if $\frac{P(Y)}{P(X)} > 1$, Y has lower energy, accept.

or $T(X \to Y) = 1$ for $P(Y) > P(X)$

on the other hand, since $E_x > E_Y$

$Y \to X$ is a tunneling process,

$\therefore T(Y \to X) = r = \frac{P(X)}{P(Y)}$

$$\therefore \quad \frac{T(Y \to X)}{T(X \to Y)} = r = \frac{P(X)}{P(Y)}$$

from detailed balance condition

$$\frac{N(X)}{N(Y)} = \frac{T(Y \to X)}{T(X \to Y)} = \frac{P(X)}{P(Y)}$$

b). if $r = \frac{P(Y)}{P(X)} < 1$, then $E_x < E_y$

$\therefore T(X \to Y) = r = \frac{P(Y)}{P(X)}$ and $T(Y \to X) =$

$$\therefore \quad \frac{N(X)}{N(Y)} = \frac{T(Y \to X)}{T(X \to Y)} = \frac{1}{r} = \frac{P(X)}{P(Y)}$$

$\therefore$ in equilibrium, $N(X) \propto P(X)$ or MC generates $P(X$

* In numerical calculation, in the beginning of the sequence generation, a strong correlation exist. One has to wait for the system to thermalize.