Chapter 2 Monte Carlo simulations

2.1 Simple sampling

This is a naive scanning of the phase space

2.1.1 Method

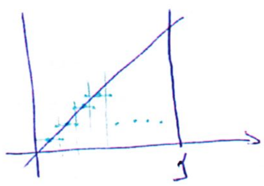
- Consider a system with N variables $\{s_1, \dots, s_N\}$ each with n possible states $\{\alpha_1, \dots, \alpha_n\}$ and energy $\mathcal{H}(s)$. Number of possible configurations is n^N.

- We want to obtain the thermodynamic average of an observable $A(s)$

$$\langle A(s) \rangle = \frac{\sum_{s_1} \dots \sum_{s_N} A(\underline{s})\, e^{-\beta \mathcal{H}(s)}}{\sum_{s_1} \dots \sum_{s_N} e^{-\beta \mathcal{H}(s)}} ; \text{ with } \beta = \frac{1}{k_B T}$$

→ Monte Carlo procedure: replace the sum over all possible states (n^N) by a random selection of M states, having all of them equal probability typically with $M \ll n^N$

Example 1: one dimensional integration



$$\int_0^1 dx\; x = \lim_{N\to\infty} \sum_{i=0}^{N-1} \frac{1}{N} \cdot \frac{(i+1/2)}{N} \simeq \sum_{i=0}^{M-1} \frac{1}{M} \cdot \frac{j(i)+1/2}{M}$$

with randomly chosen $j(i) \in [0, \dots, M-1]$

if $M=10$ (you can use google random number generator)

$j(i) = 5, 1, 8, 6, 9, 6, 1, 3, 7, 3$

$$\int_0^1 dx\; x \simeq \frac{1}{100}(49+5) = 0.54$$

other trials 0.46, 0.6, 0.48

2.1.2 Ising paramagnetic (example)

This is a system with N non-interacting spins

variables $s_i \in \{-1, 1\}$

energy $\mathcal{H}(s) = H \cdot \sum_{i=1}^{N} s_i$

H : magnetic field

Monte Carlo procedure

(i) Choose starting configuration

- Ordered case $s_i = +1 \quad \forall i = 1, \dots, N$
- Unordered case $s_i = \pm 1$ with probability 1/2

next step

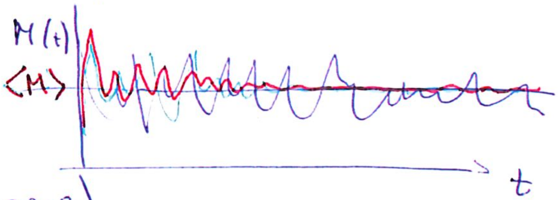
(ii) Choose a random spin 'i'

(iii) Spin-flip $s_i \longrightarrow -s_i$

(iv) Calculate the magnetization value $M = \sum_i s_i$

interpret the Monte Carlo step as time "t"

such that the $M(t)$



Average value (time average)

$$\langle M \rangle = \frac{\sum_t M(t)\, e^{-\beta \mathcal{H}(s)}}{\sum_t e^{-\beta \mathcal{H}(s)}}$$

~~!~~

Partition function - one particle $Z_1 = e^{-\beta H} + e^{\beta H} = 2 \cosh \beta H$

of N (non-interacting) particles $Z_N = Z_1^N = (2 \cosh \beta H)^N$

probability of n spins to be '+'

$$P_n = \frac{1}{Z_N} e^{-\beta H n} e^{+\beta H (N-n)} \binom{N}{n}$$

If $H=0 \rightarrow P_n^{(0)} = 2^{-N}\binom{N}{n}$

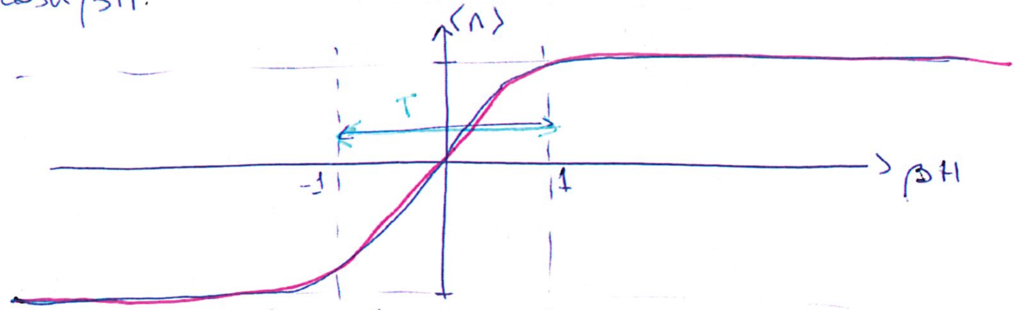
and we can rewrite $P_n = P_n^{(0)}\left(\dfrac{e^{\beta H}}{\cosh \beta H}\right)^N e^{-2\beta H n}$

the magnetization can

$$\langle M\rangle = -\left.\frac{\partial F}{\partial H}\right|_T = \langle n\rangle$$

$$F = -\frac{1}{\beta}\ln Z = -\frac{N}{\beta}\ln\left(2\cosh\beta H\right)$$

$$\langle M\rangle = \frac{N}{\beta}\,\frac{2\sinh\beta H}{2\cosh\beta H}\cdot\beta = N\tanh\beta H$$



$\left\{\begin{array}{l}\cdot \text{ large } H \text{ complete alignment}\\ T^{\circ} \text{ has a randomizing effect}\end{array}\right.$

$\Rightarrow$ Probability for $N \gg 1$; stirling's formula for $n! \simeq n(\ln n - 1)$

$$\ln P_n^{(0)} = -n\ln n - (N-n)\ln(N-n) + \underbrace{N\ln N - N\ln 2}_{\text{constant terms}}$$

we assume that: $\left.\begin{array}{l} n = \frac{N}{2}(1+x)\\ N-n = \frac{N}{2}(1-x)\end{array}\right\} \rightsquigarrow x = \dfrac{2n-N}{N}$

$$\ln P_n^{(0)} = -\frac{N}{2}\Big[(1+x)\ln(1+x) + (1-x)\ln(1-x)\Big]$$

Taylor expanding for $x \simeq 0 \rightsquigarrow \ln P_n^{(0)} \simeq -\frac{N}{2}x^2 + O(x^4)$

$$P_n^{(0)} \simeq e^{-\frac{2}{N}\left(n-\frac{N}{2}\right)^2}$$

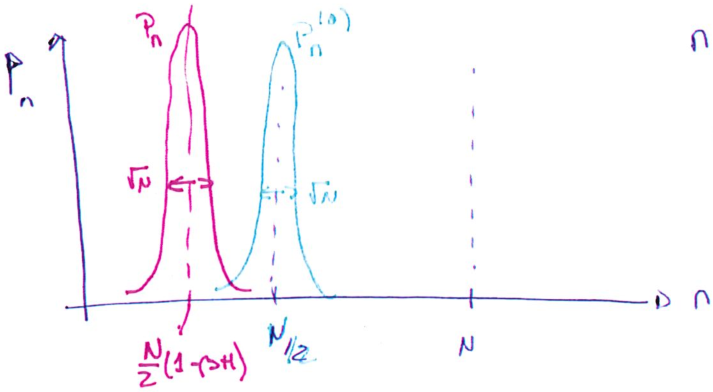
Gauss distributed around $n = N/2$

A similar expression can be obtained for $H \neq 0$

$$P_n = A \cdot \exp\left[-\frac{2}{N} \left(n - \frac{N}{2}(1-\beta H) \right)^2 \right]$$

with A - normalization factor.

displaced Gauss distribution centered at



$n = \frac{N}{2}(1-\beta H)$

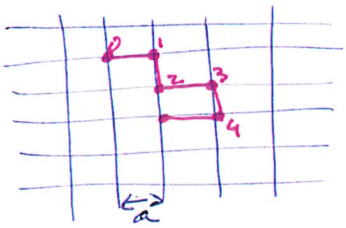
variance : : $\sqrt{N}$

- Simple sampling considers all possible configurations equally probable $\rightarrow$ this is very inefficient for the Ising paramagnetic for $|\beta H| \lesssim 1$ and $N \gg 1$
- Configurations like all aligned will basically never occur
- Mean values can not be calculated with a reasonable accuracy with a tolerable computational effort.

2.1.3 Polymer - Random walk with self-avoidance.

- Polymers are extremely long chain-like macromolecules with typically 10.000 - 100.000 monomers (repeated units)
- thermal fluctuations need to be taken into account to determine polymer configuration

- Model - 2 dimensional random walk on a grid



× We want to calculate the end-to-end distance as a function of the polymer length N

× Self-avoidance - one grid node can be occupied by at most one monomer

(a) No self-avoidance

$$\vec{R} = \sum_{i=1}^{N} a_i \quad \text{with } a_i \in a\{e_x, -e_x, e_y, -e_y\}$$

$$\langle R \rangle = 0$$

$$\langle R^2 \rangle = \sum_i \sum_j \langle a_i \cdot a_j \rangle = \sum_i \langle a_i^2 \rangle = a^2 N$$

steps are statistically independent

$$\Rightarrow \sqrt{\langle R^2 \rangle} = a N^{1/2}$$

(b) With self-avoidance

Monte Carlo procedure. Basic vectors $\begin{cases} b_1 = e_x \\ b_2 = e_y \\ b_3 = -e_x \\ b_4 = -e_y \end{cases}$

i) set $r_0 = 0$, $k = 0$

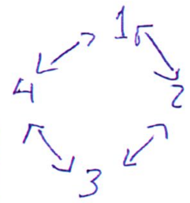
ii) Choose $j = \{1, 2, 3, 4\}$ with probability $1/4 = p$

iii) set $r_1 = b_j$ and $k = 1$

iv) Choose $j_k = \{ j_{k-1} - 1, j_{k-1}, j_{k+1} \}$; with $p = 1/3$

right, straight, left

and set $\vec{r}_k = r_{k-1} + b_{j_k}$ with $\begin{cases} b_0 \equiv b_4 \\ b_5 \equiv b_1 \end{cases}$



set $k \to k+1$

v) In case $\vec{r}_k$ reaches a previously occupied grid node $\longrightarrow$ STOP !!

to (iv)

vi) In case $k = N$ $\rightsquigarrow$ set $\vec{R} = r_N$

vii) Calculate the average value of $\langle R^2 \rangle$

Note: •) In case the algorithm stops in step (v), then the polymer of length N can not be generated.
$\rightsquigarrow$ the procedure needs to be restarted!

•) For increasing N the number of times that the process has to be restarted also increases
$\rightsquigarrow$ the algorithm also becomes inefficient.

$\square$