# Monte Carlo basics:

(talk of Markus Dutschke for the Journal Club of Theoretical Physics 3 on Nov. 4th 2013)


## *Abstract:*

This is a short introduction on MC Methods with focus on the Metropolis and Metropolis-Hasting algorithm.


## *Definition:*

> **1. Introduction.** The Monte Carlo method is generally defined as *representing the solution of a problem as a parameter of a hypothetical population, and using a random sequence of numbers to construct a sample of the population, from which statistical estimates of the parameter can be obtained.*

For our case we call:
hypothetical population = phase space
sample of the population = sample / configuration

## *Suitable Problems:*

- Mathematical integration
- distribution properties: distribution parameters, correlation coefficients
- simulation of complex processes:
  sampling over large phase spaces, minimization in large phase spaces

## *complex processes:*

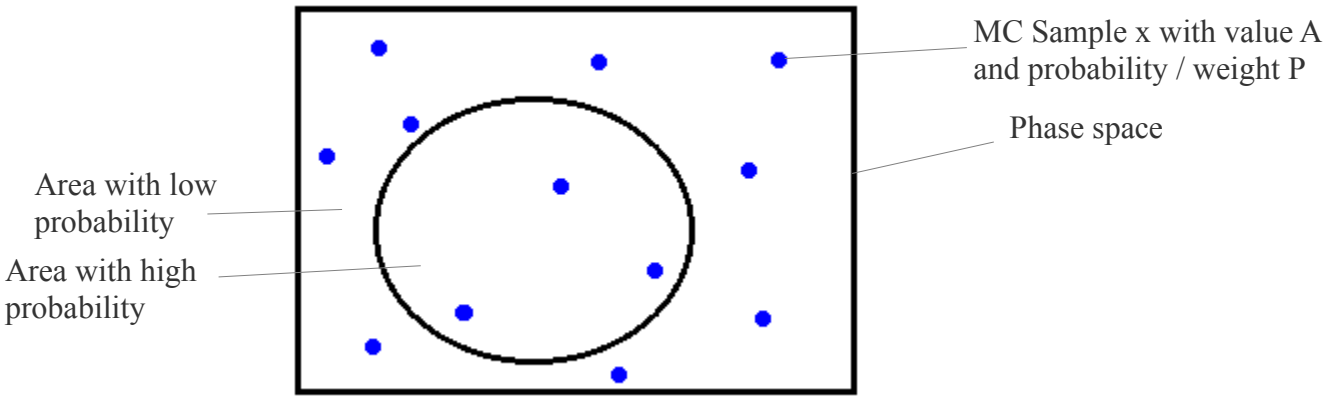
Task:
Solve a problem with a lot of different elements in a large phase space.
For example:Measure the weighted average of a quantity (and later: minimize the quantity).

$$\overline{\mathcal{A}} = \frac{\sum_x P(x)\,\mathcal{A}(x)}{\sum_x P(x)}$$

Idea:
Phase space is to big to respect all elements. Consider elements according to their importance for the task (mainly elements with high probabilities to appear).

## Simple Sampling

Example: Calculate the average value of A in a given phase space with a high probability and a low probability area.




Solution:
1) distribute random samples (x) over the hole phase space. Measure A and P
2) use the formula

$$\overline{\mathcal{A}} = \frac{\sum_x P(x)\,\mathcal{A}(x)}{\sum_x P(x)}$$

P(x): Probability to choose a configuration/sample by simple sampling
Problem: a lot of samples in an area with very low probability.

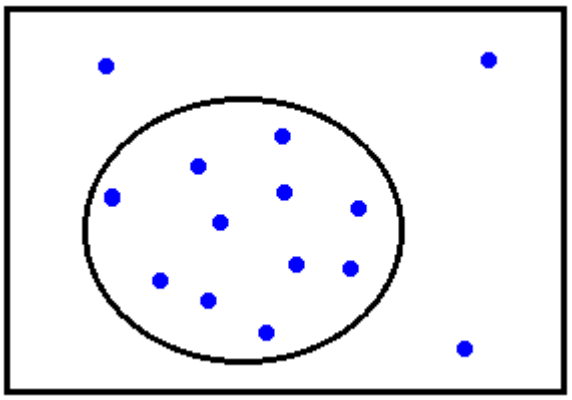
## Importance Sampling

New Solution:
1) Choose the samples according to a distribution W(x) which pays more attention to the area(s) of high probability.

2) use the formula (which pays respect to the distribution of sampling points)

Remark: A good choice for W(x) is P(x)

$$\overline{\mathcal{A}} = \frac{\sum_x P(x)\,\mathcal{A}(x)\,/\,W(x)}{\sum_x P(x)\,/\,W(x)}$$



P(x): Probability to choose a configuration/sample by importance sampling
Be carefully! This is another P(x) than that in simple sampling.

## Metropolis

Example: calculate the mean free path of non interacting particles in a box which are drive by Brownian motion

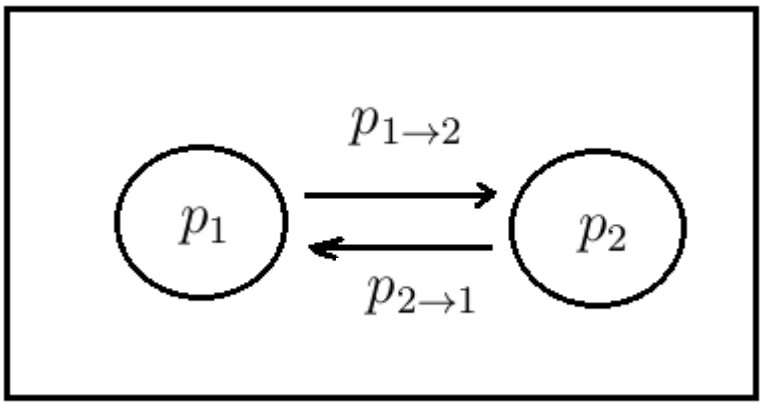
Solution:
1) start distribute particles in the box randomly
2) update: move every particle through the box; distance: random length ; direction: random
3) Accept this new configuration with the Boltzmann probability:
The Energy E is the sum of the kinetic Energy of all particles

$$p_{E_1 \to E_2} = \min\left(1; e^{-\frac{\Delta E}{kT}}\right)$$

4) check for collisions compared to the state before the update and store the path length of the particle since the last collision
5) repeat 2) to 4) very often
6) calculate the average of the saved path lengths

Explanation: Every update leads to a new distribution of the particles in a box. This distribution is one element of the very large phase space. The sequence of these elements is not predictable, but follows some rules (every particle moves according to its velocity). This is called a Markov-Chain, then. Every element of the phase space is reachable (ergodicity).
The acceptance probability ensures, that the elements of the phase space are Boltzmann distributed.
*The derivation will be shown in the next section.*

## Detailed Balance condition



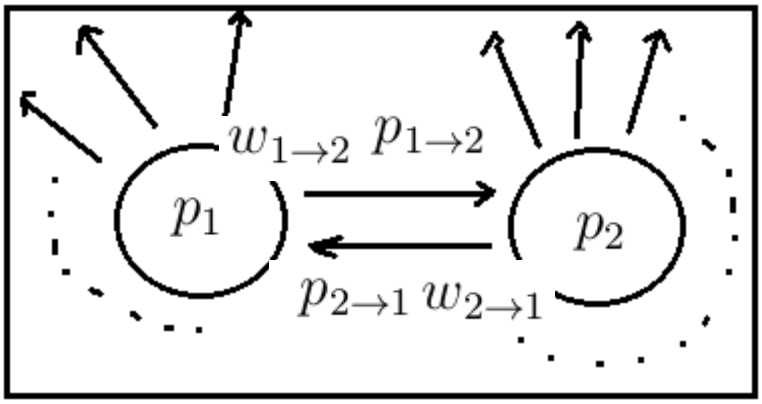

Equilibrium is achieved by the detailed balance condition:

$$p_1 p_{1\to2} \stackrel{!}{=} p_2 p_{2\to1} \qquad \text{or} \qquad \frac{p_{1\to2}}{p_{2\to1}} = \frac{p_2}{p_1}$$

The “Metropolis choice” full fills that condition:

$$\Rightarrow p_{x\to y} = \min\left(1; \frac{p_y}{p_x}\right)$$

**Detailed Balance condition for MC sampling for Metropolis(-Hasting)**




More complicated model:

proposal probability: $w_{1\to2}$

acceptance probability: $p_{1\to2}$

Detailed Balance condition:

$$p_1 w_{1\to2} p_{1\to2} \overset{!}{=} p_2 w_{1\to2} p_{2\to1}$$

$$\Rightarrow p_{x\to y} = \min\left(1; \frac{w_{y\to x} p_y}{w_{x\to y} p_x}\right)$$

**Metropolis (all proposal probabilities are the same):**

All probabilities beeing the same: $w_{x\to y} = w_{y\to x} \forall x,y$

For the "non interacting particles in a box" example this means

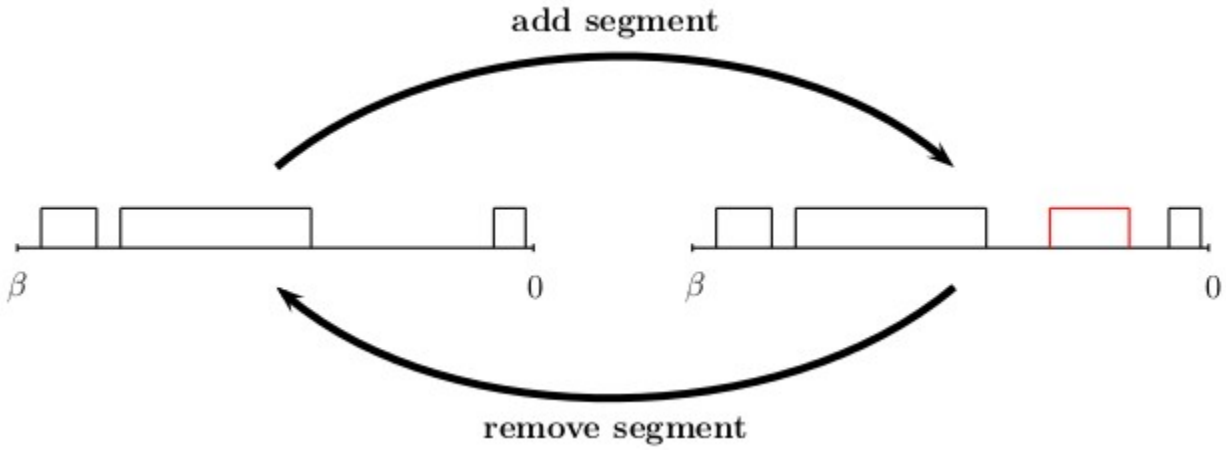
$$w((r_1,\boldsymbol{d_1});(r_2,\boldsymbol{d_2});\ldots) = w((r_1,-\boldsymbol{d_1});(r_2,-\boldsymbol{d_2});\ldots)$$

Hence it follows the acceptance probability we used in the solution of this example:

$$p_E = e^{-\frac{E}{kT}} \Rightarrow p_{E_1\to E_2} = \min\left(1; e^{-\frac{\Delta E}{kT}}\right)$$

**Metropolis-Hasting (different proposal probabilities):**

Example: basic procedure of ctqmc (continuous-time quantum Monte Carlo)
Interval between 0 and beta is divided into N parts. We can add and remove Segments on the Interval. Each Segment configuration has its own weight (x), which is calculated in a complicated way. Here we describe the add and remove process from k to k+1 Segments and the other way round.




Add segment:
1) choose a random starting point s
2) choose a random end point in (s,max]. Max is the beginning of the next Segment.
3) add segment

$$w_{\text{add}} = \frac{1}{N\,(\max - s)}$$

Remove segment:
1) choose one of the k+1 segments to remove
2) remove it

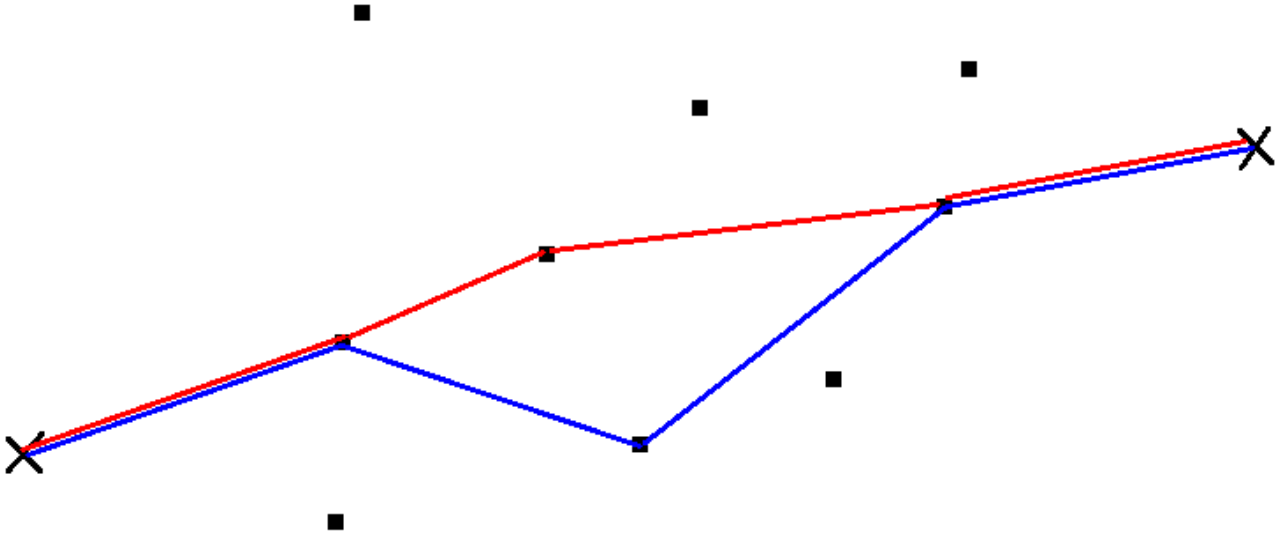
$$w_{\text{rem}} = \frac{1}{k+1}$$

$$p_{\text{add}} = \min\left(1, \frac{w_{\text{rem}}}{w_{\text{add}}}\frac{x_{k+1}}{x_k}\right) = \min\left(1, \frac{N\,(\max - s)}{k+1}\frac{x_{k+1}}{x_k}\right)$$

$$p_{\text{rem}} = \min\left(1, \frac{w_{\text{add}}}{w_{\text{rem}}}\frac{x_k}{x_{k+1}}\right) = \min\left(1, \frac{k+1}{N\,(\max - s)}\frac{x_k}{x_{k+1}}\right)$$

**Optimisation using Metropolis (*simulated annealing*):**

Example: Traveling Salesman Problem



Solution:
1) find a (bad) path from start point to end point: here blue path
2) start with some high temperature T
3) choose one node of the path and replace it with another node: → red path
4) evaluate the new path length E and except it with the (Boltzmann) probability
5) repeat 2) – 4) very often
6) decrease T and repeat 2) to 5) often
7) When you arrived at a very low temperature you are very likely to have found the shortest way

$$p_{E_1 \to E_2} = \min\left(1; e^{-\frac{\Delta E}{kT}}\right)$$

Explanation:
By also exception longer ways one can get out of local minima (blue) to get to the shortest way (green).
It is not possible to get from the blue to the green configuration without excepting longer ways.