Physica A 418 (2015) 78–87

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

An introduction to Monte Carlo methods

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HIGHLIGHTS

- We describe the main principles of Monte Carlo simulations.
- We illustrate the method with algorithms for the Ising model.
- We discuss dynamical effects such as thermalization and correlation time.

ARTICLE INFO

Article history:
Available online 25 June 2014

Keywords:
Monte Carlo simulations
Ising model
Algorithms

ABSTRACT

Monte Carlo simulations are methods for simulating statistical systems. The aim is to generate a representative ensemble of configurations to access thermodynamical quantities without the need to solve the system analytically or to perform an exact enumeration. The main principles of Monte Carlo simulations are ergodicity and detailed balance. The Ising model is a lattice spin system with nearest neighbor interactions that is appropriate to illustrate different examples of Monte Carlo simulations. It displays a second order phase transition between disordered (high temperature) and ordered (low temperature) phases, leading to different strategies of simulations. The Metropolis algorithm and the Glauber dynamics are efficient at high temperature. Close to the critical temperature, where the spins display long range correlations, cluster algorithms are more efficient. We introduce the rejection free (or continuous time) algorithm and describe in details an interesting alternative representation of the Ising model using graphs instead of spins with the so-called Worm algorithm. We conclude with an important discussion of the dynamical effects such as thermalization and correlation time.

1. Introduction

Most models in statistical physics are not solvable analytically, and therefore an alternative way is needed to determine thermodynamical quantities. Numerical simulations help in this task, but introduce another challenge: it is not possible, in most cases, to enumerate all the possible configurations of a system; one therefore has to create a set of configurations that are representative for the entire ensemble. In this section, we will illustrate our purpose with the Ising model. This is a renowned model because of its simplicity and success in the description of critical phenomena [1]. The degrees of freedom are spins $S_i = \pm 1$ placed at the vertex i of a lattice. This lattice will be square or cubic for simplicity, with edge size L and

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http://dx.doi.org/10.1016/j.physa.2014.06.014
0378-4371/

dimension D. Thus, the system contains $N = L^D$ spins. The Hamiltonian of the Ising model is:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j, \tag{1}$$

where the summation runs over all pairs of nearest-neighbor spins $\langle ij \rangle$ of the lattice and J is the strength of the interaction. The statistical properties of the system are obtained from the *partition function*:

$$Z = \sum_{\mathcal{C}} \mathrm{e}^{-\beta E(\mathcal{C})}, \tag{2}$$

where the summation runs over all the configurations $\mathcal{C}$. The energy of a configuration is denoted by $E(\mathcal{C})$. Here, $\beta \equiv 1/(k_B T)$ is the inverse temperature (temperature T and Boltzmann constant k_B). The Ising model displays a second-order phase transition at the temperature T_c, characterized by a high temperature phase with an average magnetization zero (disordered phase) and a low temperature phase with a non-zero average magnetization (ordered phase). The system is exactly solvable in one and two dimensions. For $D \geq 4$, the critical properties are easily obtained by the renormalization group. In three dimensions no exact solution is available. Even a $3D$ cubic lattice of very modest size $10 \times 10 \times 10$ generates $2^{1000} \approx 10^{301}$ configurations in the partition function. If we want to obtain e.g. critical exponents with a sufficient accuracy, we need sizes that are at least an order of magnitude larger. An exact enumeration is a hopeless effort. *Monte Carlo simulations* are one of the possible ways to perform a sampling of configurations. This sampling is made out of a set of configurations of the configuration space that contributes the most to the averages, without the need of generating every single configuration. This is referred to as *importance sampling*. In this sampling of the configuration space, it is important to choose the appropriate Monte Carlo scheme to reduce the computational time. In that respect, the Ising model is interesting because the different regimes in temperature lead to the development of new algorithms that reduce tremendously the computational time, specifically close to the critical temperature.

We will start these notes by introducing two important principles of Monte Carlo simulations: detailed balance and ergodicity. Then we will review different examples of Monte Carlo methods applied to the Ising model: local and cluster algorithms, the rejection free (or continuous time) algorithm, and another kind of Monte Carlo simulations based on an alternative representation of the spin system, namely the so-called Worm algorithm. We continue with discussing dynamical quantities, such as the thermalization and correlation times.

2. Principles of MC simulations: ergodicity and detailed balance condition

The basic idea of most Monte Carlo simulations is to iteratively propose a small random change in a configuration C_i, resulting in the trial configuration C^t_{i+1} (the index "t" stands for trial). Next, the trial configuration is either accepted, i.e. $C_{i+1} = C^t_{i+1}$, or rejected, i.e. $C_{i+1} = C_i$. The resulting set of configurations for $i = 1 \ldots M$ is known as a Markov chain in the configuration space of the system. We define $P_A(t)$ as the probability to find the system in the configuration A at the time t and $W(A \to B)$ the transition rate from the state A to the state B. This Markov process can be described by the master equation:

$$\frac{\mathrm{d}P_A(t)}{\mathrm{d}t} = \sum_{A \neq B} \left[P_B(t) W(B \to A) - P_A(t) W(A \to B) \right], \tag{3}$$

with the condition $W(A \to B) \geq 0$ and $\sum_B W(A \to B) = 1$ for all A and B. The transition probability $W(A \to B)$ can be further decomposed into a trial proposition probability $T(A \to B)$ and an acceptance probability $A(A \to B)$ so that $W(A \to B) = T(A \to B) \cdot A(A \to B)$. A proposed change in the configuration is usually referred to as a Monte Carlo move. Conventionally, the time scale in Monte Carlo simulations is chosen such that each degree of freedom of the system is proposed to change once per unit time, statistically.

The first constraint on this Markov chain is called *ergodicity*: starting from any configuration C_0 with nonzero Boltzmann weight, any other configuration with nonzero Boltzmann weight should be reachable through a finite number of Monte Carlo moves. This constraint is necessary for a proper sampling of the configuration space, as otherwise the Markov chain will be unable to access a part of configuration space with a nonzero contribution to the partition sum.

Apart from a very small number of peculiar algorithms, a second constraint is known as the *condition of detailed balance*. For every pair of states A and B, the probability to move from A to B, as well as the probability for the reverse move, are related via:

$$P_A \cdot T(A \to B) \cdot A(A \to B) = P_B \cdot T(B \to A) \cdot A(B \to A). \tag{4}$$

The meaning of this condition can be seen in Eq. (3): a stationary probability (i.e. $\mathrm{d}P_A/\mathrm{d}t = 0$) is reached if each individual term in the summation on the right hand side cancels. This prevents the Markov chain to be trapped in a limit cycle [2]. This is a strong, but not necessary, condition. We mention that generalizations of Monte Carlo process that do not satisfy detailed balance exist. The combination of ergodicity and detailed balance assures a correct algorithm, i.e., given a long enough time, the desired distribution probability is sampled.

The key question in Monte Carlo algorithms is which small changes one should propose, and what acceptance probabilities one should choose. The trial proposition and acceptance probabilities have to be well chosen so that the probability of