# The Monte Carlo Model and Its Application

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*Abstract:* This research mainly investigated the Monte Carlo model through literature review and case analysis. This research provides an example of the area of a circle to quickly understand what a Monte Carlo model is. Through Monte Carlo, this paper introduced some other algorithms based on it, such as Markov chain, Monte Carlo Markov chain algorithm and Metropolis algorithm. In addition, the Ising model was introduced and it was found that the model can calculate the energy change corresponding to different probabilities of spin acceptance or rejection flip using the Boltzmann distribution at the same temperature. The main objective of this research is that most Ising models occur in high-dimensional states, changing the spin will affect the adjacent spins, and the difficulty of calculating the energy changes increases dramatically with increasing dimensions. Research has found that Monte Carlo methods enable Ising model problems in high-dimensional or complex interactions to be effectively solved through Monte Carlo simulations. Through extensive random sampling and statistical processing, Monte Carlo simulations can estimate the transition behavior of each spin.

*Keywords:* Monte Carlo, Markov Chain, Metropolis Algorithm, Ising Model, Boltzmann Distribution.

## 1. Introduction

Monte Carlo method is a computational method based on random sampling and statistical analysis of numerical values. One of the most typical applications is the Ising model, which is one of the classic models in physics mainly used to describe the interaction between magnetic changes and spin states. In known low dimensional Ising models, the energy changes caused by spin can be analytically solved through calculations. However, for high-dimensional systems or systems with complex interactions, it is difficult for people to calculate. Therefore, Monte Carlo simulation provides a computerized method to solve this problem by estimating the phase transition behavior of the system in thermodynamic properties through random sampling. Therefore, Monte Carlo algorithm plays an important role in the calculation and research of Ising models in high-dimensional or complex states.

This research mainly introduced the Monte Carlo model and some models based on it, among which this research mainly introduced the Metropolis algorithm. This research analyzes how Monte Carlo is applied in the Ising model using the Metropolis method.

This research has broad application value in materials research. By using a Monte Carlo algorithm in the Ising model, people can better simulate self-rotating phase transitions and critical phenomena,

and better predict the performance of materials under different temperatures and external conditions. This has significant implications for the development of new magnetic materials and smart materials.

## 2.　Monte Carlo Simulation

### 2.1.　Introduction to Monte Carlo Method

Monte Carlo is a common sample application of mathematics, and it is also known as Monte Carlo method. The calculation method uses random numbers and is based on probability and statistical theory. This research has chosen the version of the book: Monte Carlo Methods, Volume 1: Basics for explanation here [1].

Monte Carlo simulation is a method of solving problems through random sampling, which obtains possible results through multiple random generations to simulate the behavior of complex systems or estimate unknown variables. Through a large number of random experiments, Monte Carlo simulation can provide approximate solutions to problems, and the accuracy of the results increases with the number of experiments.

The development of modern computers has made Monte Carlo simulation a useful computational method because it can generate large amounts of random data and perform complex operations quickly.

### 2.2.　Typical Applications of Monte Carlo Methods

A typical application of Monte Carlo method is to calculate the area of a circle. The calculation principle is to define a unit square and a unit circle within it, randomly scatter points within the unit square, and then calculate the ratio of the number of points falling within the unit circle to the total number of points to approximate the area of the circle [2].

The advantage of this method is that it does not require knowledge of the mathematical formula of a circle, and through a large number of random experiments, the results calculated by Monte Carlo can be made close to real values.

Actual application can be calculated through the following steps:

A. Create a square with a side length of 2 at the origin position, with its center at the origin, and define a circle with a radius of 1 in it.

B. Randomly generate a large number of points within the square, and control the range of the large number of points between +1 and -1.

C. Determine whether each point is within the circle.

D. Count the number of randomly generated points within a circle and calculate their ratio to the total number of points falling, in order to estimate the area of the circle.

Although this method may seem simple, it provides a new approach to solving complex mathematical problems. Especially after the development of computer technology, it is possible to create countless random numbers through Python tools to achieve a large number of random experiments, thus obtaining more accurate results.

The application of Monte Carlo method is not limited to calculating the area of geometric shapes, but also includes multiple fields such as simulating physical processes and optimization problems.

## 3.    Ising Model

### 3.1.   Introduction to Ising Model

The Ising model is a classic example of using Monte Carlo methods to simulate physical processes in physics. In the application of the Ising model, Monte Carlo method is an important numerical simulation technique used to study the phase transition and thermodynamic properties of the system.

The principle of the Ising model is to generate a series of random elements within a specified range and flip one of their spins, calculate the energy difference of the system before and after each flip, the change in computing power, total energy, and magnetization. Because the spin of each element can be +1 or -1, a randomly generated dataset composed of many elements has many combinations of spin arrangements. Therefore, it is very difficult to analyze numerical values in complex situations.

In the Ising model, the complexity of the model, usually refers to the difficulty in handling or analyzing problems under standard conditions, which also increases the complexity of the system. For example, the Ising models commonly studied occur in one dimension. However, in higher dimensional Ising models, if the spin of any element is changed, the number of adjacent affected elements will significantly increase and the scale in dynamic space will also sharply increase, leading to an increase in system complexity and computational complexity [3]. Therefore, Monte Carlo methods are used to approximate these complex problems through random sampling.

The purpose of using Monte Carlo method is to analyze the variation energy and magnetic field strength of Ising model, and help understand the microscopic mechanism of spin. The Monte Carlo method enables the Ising model problem under high-dimensional and complex interactions to be effectively solved through numerical simulations. Through extensive random sampling and statistical processing, Monte Carlo simulation can approximate the phase transition behavior and thermodynamic properties of the Ising model.

### 3.2.   The Boltzmann Distribution

The Boltzmann distribution is a probability distribution in statistical physics used to describe the probability distribution of various energy states at thermodynamic equilibrium. It indicates that the probability of energy in a system in thermodynamic equilibrium is proportional to the energy of that state, and the lower the energy, the higher the probability of occurrence, as shown in the following formula [4]:

$$p \sim e^{-\frac{\triangle E}{kT}} \qquad (1)$$

This is the explanation for the Boltzmann distribution in this research. The P in the formula represents probability, $\triangle E$ is the change of total energy and T is thermodynamic temperature. The k in the formula represents the Boltzmann constant. This formula represents P is proportional to the index e contain E and T. The Ising models in this study obtain different probabilities by varying the energy changes at the same temperature.

In the Ising model, each spin accepts or rejects flipping based on the probability of the Boltzmann distribution, simulating the system state.

### 3.3.   Markov Chain Monte Carlo Method, Markov Chain and Metropolis Algorithm

Apart from Monte Carlo method, Markov Chain Monte Carlo method (MCMC) is also a random sampling method. This method introduces Markov process into Monte Carlo simulation, achieving dynamic simulation of sample distribution changing with the progress of the simulation, which compensates for the limitation of traditional Monte Carlo methods that can only simulate statically.

This method is commonly used to generate samples from complex probability distributions, especially when direct sampling is not possible.

Similar to the Markov Chain Monte Carlo method (MCMC) is the Markov chain. Markov chain is a stochastic process in which the change of each state depends only on the current state and is independent of previous states. This property is called memorylessness. It is used to simulate the state changes of a system over time, ultimately achieving a stationary distribution. This is the foundation of the Metropolis algorithm. For example, in the Ising model, changes in the current spin configuration are only related to the current spin state, and do not depend on its previous change.

In MCMC algorithm, the sample generation process is a Markov chain. Therefore, in conclusion, compared to Markov Chain Monte Carlo Method (MCMC) and Markov Chain, Markov Chain is a mathematical tool or model, while MCMC is a computational technique based on Markov Chain used for sampling from complex probability distributions.

For physical systems, such as Ising model, through sufficient iterations, the MCMC method will stabilize the state distribution, achieving the equilibrium distribution of the system. The goal of a Markov chain is to gradually approach a target distribution of system states through continuous state transitions (usually the Boltzmann distribution).

The Metropolis algorithm is also a Monte Carlo method based on Markov chains, used for sampling from complex probability distributions and widely used in simulations in statistical physics. Its purpose is to simulate the thermodynamic behavior of complex systems through random sampling [5].

The Metropolis algorithm is widely used in various physical problems, such as phase transition research, molecular dynamics simulations in materials science, and critical point analysis of phase transitions in Ising model. Its advantage is that even in complex high-dimensional systems, it can still effectively generate statistical equilibrium states of the system. In the Ising model, the main goal of the Metropolis algorithm is to construct a Markov chain so that the equilibrium distribution of the chain is exactly the desired target distribution [6]. At each step, the algorithm randomly generates a new state based on the current state and determines whether to transition to the new state through an Acceptance Rejection Criterion.

### 3.4. Practical Application of Ising Model

This research mainly studies how to calculate a two-dimensional Ising model. Firstly, investigate how to establish the total energy and magnetization of an Ising model at a specific temperature.

The main algorithm steps are:

A. Create a matrix and randomly assign an initial value (+1 or -1 random distributions) to the spin of each element in the sample.

B. Calculate M, which means the sum of the total sample set (magnetization)

C. Calculate E, which means the total energy of spins in the sample:

For two adjacent elements, if their initial values are the same, they will receive an energy of - k; If the initial values of two spins are different, then the energy of +k will be obtained. Each spin only generates energy for four adjacent spins. Next, calculate the sum of energy generated by the spin of each pair of adjacent elements in the entire sample set.

The M and E calculated in this way are the thermodynamic values obtained under the arrangement of the element combination. Next, let's find the percentage of elements that satisfies the Markov chain. The first step is to randomly change the assignment of one spin.

The main algorithm steps are:

A. Randomly select an element and change its spin direction (from+1 to -1 or from -1 to+1).

B. Calculate the energy change of the total sample before and after flipping the element

C. Determine whether to accept or reject flipping of the element:

    i. If the energy change satisfies the acceptance condition (such as delta E<=0 or random probability), then flip the spin of the point and update the total energy and magnetization, then the element accepts the flip.

    ii. If it is not satisfied, the element rejects to flip.

    D. Repeat the above steps to calculate and output the percentage of points that accept flipping.

## 4.    Conclusion

This article mainly studies the Monte Carlo model and some Monte Carlo based algorithms, such as the Metropolis algorithm, Markov chain, and Monte Carlo Markov chain. It specifically introduces the application of the Metropolis algorithm in the Ising model, and studies that the probability of each spin changing direction under different energy changes in the Ising model at the same temperature exhibits a Boltzmann distribution. In addition, this research specifically lists the methods of changing the energy change caused by a random spin in the Ising model in a two-dimensional state, and the probability of each spin change can be obtained through the energy change. Therefore, the Monte Carlo method can be used to estimate the phase transition behavior of the Ising model in high-dimensional or complex systems.

    This research did not provide a detailed introduction to the various interactions in the Ising model. In practical applications, the Ising model may adopt several different spin interaction processes. More complex relationships are more applicable in real life. Therefore, the future research areas of the Ising model can focus on complex spin interactions, such as long-range interactions, which can be achieved using Monte Carlo methods.

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