

# Principle and Applications of Monte-Carlo Simulation in Forecasting, Algorithm and Health Risk Assessment

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**Abstract.** Monte Carlo simulation, as a technique to reverse parameters by random sampling in known data, is widely used in many fields such as finance, computer and engineering. While introducing the basic concepts and related principles of Monte Carlo simulation, this paper will focus on three new applications of Monte Carlo simulation in electricity price prediction, algorithm and health risk assessment. The limitations and future development of the Monte Carlo simulation are discussed later. Future research should solve the defects of Monte Carlo simulation with long computing consumption time, lack of evaluation method and strict sampling requirements, and enhance the adaptability of this method by combining the problems worth research in various fields. This paper hopes to provide the reader with the relevant background knowledge of Monte Carlo simulations to facilitate the application of Monte Carlo simulation to complex problems in more domains. Overall, these results shed light on guiding further exploration of applications based on Monte Carlo Simulations.

**Keywords:** Monte Carlo simulation; health risk assessment; MCMC; electricity price forecasting.

## 1. Introduction

After the French scientists Comte de Buffon and the "Buffon's needle", the Monte Carlo method was initially systematically applied in the Manhattan Project. John von Neumann and Stanislaw Ulam studied the properties of neutron diffusion in nuclear weapons by repeated random sampling, and named this method after a casino in Monaco [1]. Monte Carlo methods were gradually used to study problems in other fields of physics in the mid-to-late 20th century, such as particle transport and Boltzmann Transport Equation [2, 3]. In recent years, in many fields such as medical, engineering, aerography, finance, computer science, statistics, the idea of random sampling in the Monte Carlo method has been combined with statistical modeling to form a new model for estimation, sampling and optimization called Monte Carlo simulation [4]. Monte Carlo simulations are widely used not just because their predictions of failures, cost and progress overruns are ordinarily superior to human intuition or alternative analytic methods. As a technique supported by a lot of mathematical and statistical knowledge, Monte Carlo simulation can reduce complex models to a basic set of events and interactions between them to implement on a computer, and its parallelizable makes it greatly reduce the computation time. Its inherent randomness is crucial for the simulation of real-life stochastic systems and the deterministic numerical computation [5]. Therefore, Monte Carlo simulation is a method that cannot be ignored and is worthy of intensive study, especially since it has shone in many important academic fields.

In financial engineering, many problems can be summarized as an estimate of a certain value. Typically, this value is converted into the expectation of a complex random variable after which the behavior is modeled as a random process, while Monte Carlo simulations that are easy to use and convergence rates generally are generally not limited by the dimensions of the problem are often used to estimate expectations [6]. In the field of operations and optimization, a several stage simulation techniques that could solve the travel salesperson problem (TSP) called Multistage Monte Carlo optimization was designed to seek for optimal solutions by sampling distributions in the space of feasible solutions to various optimization problems [7]. Monte Carlo simulation methods have also been used to study the thermodynamic properties of model systems with a certain multiple degree of freedom, by randomly sampling the phase space of the system and using computer generation of a

series of random types without changing parameters [8]. In the field of statistics, SIMR is a very flexible method based on Monte Carlo simulation and is often used to analyze the power estimation of two-stage models with hierarchical structured data [9].

This paper would detailly introduce the recent innovative applications of Monte Carlo simulation in forecasting, algorithm and risk assessment, summarize the advantages and current limitations of these applications and suggest possible future directions for Monte Carlo simulation. It is hoped that this paper will help readers to understand and grasp the research and development process in this field from a macro perspective, and also provide readers with relevant background knowledge to promote the application of Monte Carlo simulation of complex problems in more fields.

## 2. Basic Descriptions of MC

Although Monte Carlo simulations are often implemented in different ways in different fields, most of them follow three steps, construct a system composed of the probability density function, repeat the random sampling and get the results of each sampling, and analyze the results [4]. First, the distribution of the input data with the mean and variance should be determined, and then a system that can get the desired results was built. Afterwards, a sample is randomly drawn from a random variable with a PDF and its mean is calculated. According to the law of large numbers, this value can be taken as the estimator of the expected value of the population when the sample size approaches infinity [4]. The expected value of the population would be regarded as input to the system with more complex results. To obtain valid results, the sampling method should be completely random, but allowing the computer to generate pseudo-random series of any complex distribution is time-consuming. Therefore, in most cases, researchers need to convert the samples from simple distributions that easily obtained from the computer, such as uniform distribution and normal distribution, into the samples from required complex distribution [10]. The most common uniform random number generation method came from the Monte Carlo roulette game. In the computer, it is done through a mixed congruential relationship below:

$$R_{k+1} = (aR_k + c) \text{ mod } m \quad (1)$$

where  $R_k$  represents the  $k$ th number in the sequence of generated random numbers,  $a$  and  $c$  are non-negative integer parameters, and  $R_{k+1}$  is the remainder divided by the integer  $m$ . Sequences generated with the above expression is periodic with period  $p$  that less than  $m$ , so are actually deterministic, also known as pseudo-random numbers. When  $a$ ,  $c$ , and  $m$  are adjusted, the period  $p$  can become large and these numbers can pass randomness tests. Thus, the sequence of generated random numbers can be used as a random number. Then, this paper will introduce how to convert samples from uniform distribution into samples from exponential distribution by inversion method. The exponential distribution's pdf and cdf are as follows:

$$f(x) = \lambda e^{-\lambda x} \quad (2)$$

$$F(x) = 1 - e^{-\lambda x} \quad (3)$$

where  $\lambda$  is constant. Assuming that  $t$  is a sample from uniform distribution, there is an  $x$  belonging to the exponential distribution satisfying the following expression

$$F(x) = u \quad (4)$$

and then

$$x = F^{-1}(u) = -\frac{\ln(1-u)}{\lambda} \quad (5)$$

The method can be similarly extended to cdf with inverse functions

### 3. Applications

#### 3.1. Electricity Price Forecasting

As the electricity market gradually opens up and leaves government control, electricity has become a common commodity in energy and related industries. Because it can reflect the relationship between supply and demand, Short-term, medium-term and long-term EPFs (electricity price forecasting) has become an important part of the decision of competitors in the electricity market [11]. New changes in the energy industry, such as intensifying market competition, aging infrastructure, the introduction of smart grid and the development of renewable energy, greatly enhance the importance of probabilistic forecasting to the planning and operation of energy systems. According to the paper of Jakub Nowotarski and Rafal Weron, historical simulation, distribution-based probabilistic forecasts, boot strapped PIs and Quantile Regression Averaging (QRA) have been applied in the field [12]. In fact, Monte Carlo simulation, as a non-primary method or a phased method, is used to predict the mid-term hourly electricity price through the spatial interpolation technology in 2015 [13]. This article will describe an adaptive longterm electricity price forecasting model. The electricity price is modeled as

$$\log(P_t) = f(t) + X_t \quad (6)$$

where  $P_t$  is the price of electricity (US\$/MWh),  $f(t)$  is the deterministic seasonal component with regression to mean levels,  $X_t$  is the random part of the model. Then model  $f(t)$  by trigonometric functions and model  $X_t$  by mean reverting

$$f(t) = s_1 \sin(2\pi t) + s_2 \cos(2\pi t) + s_3 \sin(4\pi t) + s_4 \cos(4\pi t) + s_5 \quad (7)$$

$$dX_t = (\alpha - \kappa X_t)dt + \sigma dW_t + J(\mu_j, \sigma_j)d\Pi(\lambda) \quad (8)$$

where  $s_i$  are constant and  $t$  is annualized time factors.  $\alpha$  and  $\kappa$  are the mean-reversion parameters, and  $\sigma$  is the volatility.  $W_t$  is a standard Brownian motion. The size and intensity of jumps are represented as normally distribution  $J(\mu_j, \sigma_j)$  with mean and standard deviation, and Poisson process  $\Pi(\lambda)$  with parameter  $\lambda$ . Taking the date and the corresponding electricity price as input and find  $\log(P_t)$  with  $t$ . After the  $s_i$  was determined by the least squares method, the deterministic seasonal part was removed from Eq. (6). To discretize the  $X_t$ , one assumes the jump of price as a Bernoulli process (most one jump per day) with probability  $(1 - \lambda\Delta t)$  and probability  $\lambda\Delta t$ :

$$X_t = \alpha\Delta t + (1 - \kappa\Delta t)X_{t-1} + \sigma\xi \quad (9)$$

$$X_t = \alpha\Delta t + (1 - \kappa\Delta t)X_{t-1} + \mu_j + \sigma_j\xi_j + \sigma\xi \quad (10)$$

where  $\xi$  and  $\xi_j$  are independent standard normal random variables. The density function of  $X_t$  is

$$f(X_t|X_{t-1}) = (\lambda\Delta t)[2\pi(\sigma_j^2 + \sigma^2)]^{-\frac{1}{2}}e^{N1} + (1 - \lambda\Delta t)(2\pi\sigma^2)^{-\frac{1}{2}}e^{N2} \quad (11)$$

$$N1 = \frac{-(X_t - \alpha\Delta t - (1 - \kappa\Delta t)X_{t-1} - \mu_j)^2}{2(\sigma_j^2 + \sigma^2)} \quad (12)$$

$$N2 = \frac{-(X_t - \alpha\Delta t - (1 - \kappa\Delta t)X_{t-1})^2}{2\sigma^2} \quad (13)$$

The parameter  $\theta = \{\alpha, \kappa, \mu_j, \sigma_j^2, \sigma^2, \lambda\}$ , then minimize the negative log likelihood function:

$$\min\theta - \sum_t^T \log[f(X_t|X_{t-1})] \quad (14)$$

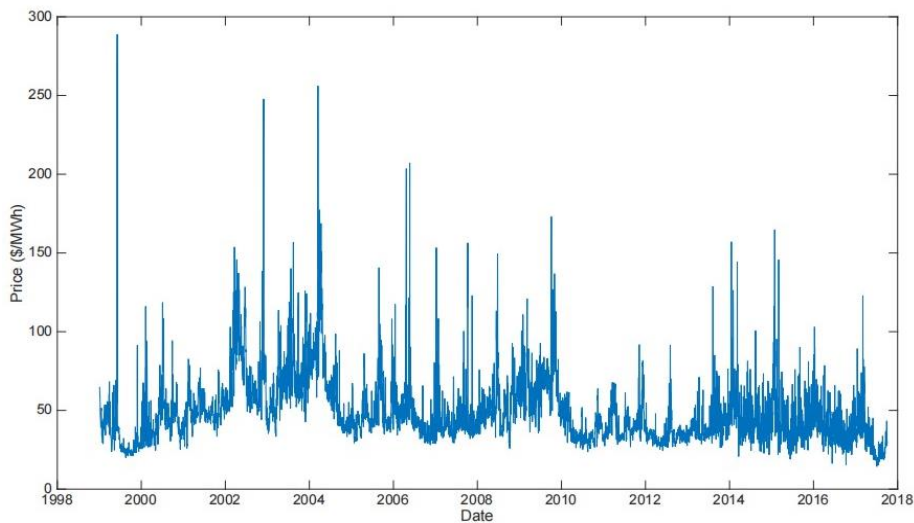
With constraints

$$1 - \kappa\Delta t > 1 \quad (15)$$

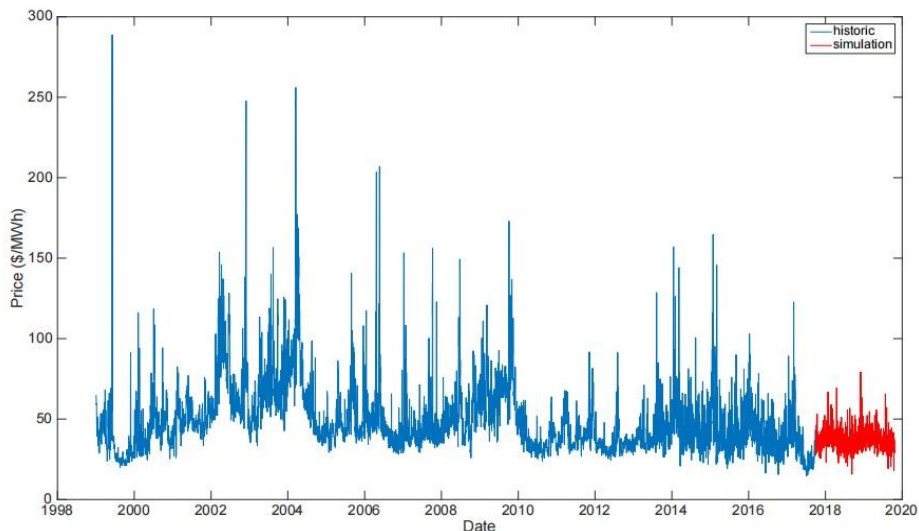
$$\sigma_j^2, \sigma^2 > 0 \tag{16}$$

$$0 \leq \lambda \Delta t \leq 1 \tag{17}$$

The resulting parameters and models can be used for Monte Carlo simulations (seen from Fig. 1 and Fig. 2). Deterministic seasonal part was added to simulated paths after 10000 simulations. The paper examined the range of predictions at 2,5, and 10 years, respectively. For the 2-year forecast period, the average price was 38.04 US \$ / MWh, while the historical average price was 49.18 US \$ / MWh, demonstrating the stability and accuracy of the model. The validation of the accuracy of the model is not satisfactory. Splitting the training set and test sets, such as predicting the 2017-2018 average electricity prices through data from 1998 to 2016, are perhaps better ways to demonstrate the accuracy and adaptability of the model [11].



**Fig. 1** Historic electricity prices.



**Fig. 2** The electricity price forecast for two years

### 3.2. Markov Chain Monte Carlo

A special Monte Carlo method for obtaining distribution information which is often used to estimate the posterior distribution in Bayesian inference is called Markov Chain Monte Carlo (MCMC). The two parts of the name each contain a property: Monte Carlo shows that it is still used to estimate the distribution of the data and the relevant information through random sampling, while the Markov chain means that these random samples are generated by particular sequences where each item is related only with the previous one [14]. The common process of Bayesian inference is using

the information provided by the observed data to update the prior state of beliefs to the posterior state of beliefs. One point of MCMC advantages over analytical tests is that in some cases, MCMC is able to estimate certain parameters of the posterior distribution that cannot be computed directly [15]. In practice, however, computers will spend a large amount of time to calculate these parameters, the reason being that to get precise results, MCMC algorithms usually need to process all the data repeatedly in iterations [15]. A strategy for splitting the data was proposed in 2018. The overall posterior was estimated by running the corresponding independent MCMC algorithm on the postbatch data to spread the computational burden across multiple individual computer cores to recombine the subposterior [16]. How to effectively partition the data and quantify the approximate accuracy of these merging processes becomes a new problem. At present, the most popular algorithm to reduce the computation time is a class of extendible stochastic gradient MCMC (SGMCMC) methods based on sub-sampling.

Before the SGMCMC is introduced, its basic theory the Langevin diffusion should be understood. Assume  $\theta \in \mathbb{R}^d$ , the target density  $\pi(\theta)$  to be sampled is directly proportional to the  $\exp\{-U(\theta)\}$ , and  $U(\theta)$  is potential function which is continuous and differentiable almost everywhere.

$$U(\theta) = \sum_{i=1}^N U_i(\theta) \tag{18}$$

$$U_i(\theta) = -\log f(y_i|\theta) - \frac{1}{N} \log p(\theta) \tag{19}$$

The method to generate samples from  $\pi(\theta)$  is to simulate a stochastic process with  $\pi$  as a stationary distribution, one of the most prevalent examples is MCMC. Langevin diffusion is represented by stochastic differential equations under mild regularity conditions:

$$d\theta(t) = -\frac{1}{2} \nabla U(\theta(t)) dt + dB_t \tag{20}$$

$\nabla U(\theta(t))$  is the drift term, and  $B_t$  represents the d-dimensional Brownian motion. When the time interval  $h$  is greater than 0,

$$\theta(t+h) \approx \theta(t) + \sqrt{h}Z - \frac{h}{2} [\nabla U(\theta(t))] \tag{21}$$

where  $Z$  is the vector consisting of  $d$  independent standard random variables meeting a standard Gaussian distribution. This is also the Euler approximation that is commonly used in practice to generate samples. The more common algorithm are Metropolis-adjusted Langevin Algorithm and unadjusted Langevin algorithm. Examples of sampling from a Gaussian distribution are presented in Fig. 3 (plotted over the bivariate Gaussian target). Next comes the introduction of the SGMCMC.

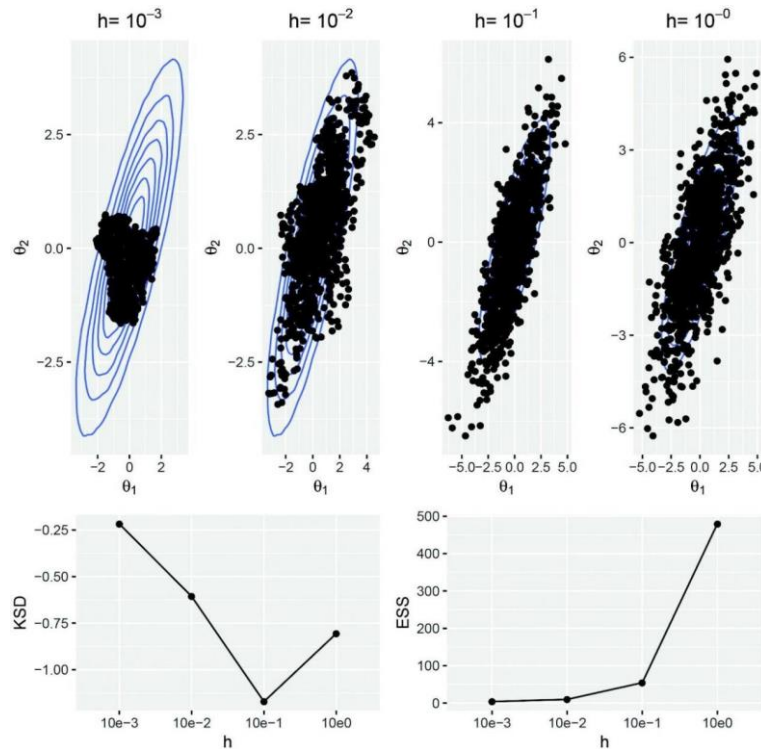
Diffusion processes with  $\pi$  as the stationary distribution can be approximated from one of the diffusion processes using similar ideas. This paper introduces a general approach. First, assume a  $\zeta$  containing  $\theta$  as a general state (possibly contains auxiliary variables), whose general stochastic differential equation is as follows:

$$d\zeta = \sqrt{\mathbf{D}(\zeta)} dB_t + \frac{1}{2} \mathbf{b}(\zeta) dt \tag{22}$$

It contains the drift component ( $\mathbf{b}(\zeta)$ ) and a positive semi-definite diffusion matrix ( $\mathbf{D}(\zeta)$ ). After, define a function  $H(\zeta)$  whose natural exponential function is integrable, and  $\mathbf{Q}(\zeta)$  is an skew-symmetric curl matrix. When  $\mathbf{b}(\zeta)$  satisfies the following two equations, the stationary distribution of (22) is proportional to the  $\exp\{-H(\zeta)\}$ :

$$\mathbf{b}(\zeta) = -[\mathbf{D}(\zeta) + \mathbf{Q}(\zeta)] \nabla H(\zeta) + \Gamma(\zeta) \tag{23}$$

$$\Gamma_i(\zeta) = \sum_{j=1}^d \frac{\partial}{\partial \zeta_j} (D_{ij}(\zeta) + Q_{ij}(\zeta)) \tag{24}$$



**Fig. 3** Samples generated from the Langevin dynamics.

To approximate sampling from the diffusion, using the same discretization of the continuous-time dynamics, to calculate  $\zeta_{t+h}$  by  $\zeta_t$ . However,  $Z$  in the new equation fits a normal distribution with mean 0 and variance  $\mathbf{D}(\zeta_t)$ . A general class of SGMCMC algorithms can be derived by replacing gradient estimate  $\nabla H(\zeta)$  by unbiased estimate  $\widehat{\nabla} H(\zeta)$ . The diffusion  $D$  and curl matrices  $Q$  can take many forms and vary by the SGMCMC algorithms. The choice would affect the convergence efficiency of the MCMC sampler. A diagnostic test based on Stein’s discrepancy for SGMCMC is proposed to assess the accuracy of a sample of a value approximates a distribution. The article does not evaluate the advantages and disadvantages of various types of SGMCMC, but suggests some development directions e. g. algorithms, general theoretical results and tuning techniques.

### 3.3. Health risk assessment

Soil is not only an important environmental medium, but also a potential route for human exposure to pollutants. Heavy metals are released from natural processes and man-made sources, and passing through the food chain after entering agricultural soil increases potentially adverse health risks. In recent years, human agricultural activities have led to an increase in the content of heavy metals in the soil, and their harm is increasingly concerned by the global public [17]. Similarly, parks play an important role in residents’ daily leisure, outdoor sports, and social and urban ecosystems. However, park soil as an environmental medium, may also be a potential way for citizens to be affected by pollutants such as heavy metals [18]. These heavy metals can be transferred to humans through ingestion, inhalation and skin absorption pathways, especially in children and the elderly [19]. They are more vulnerable to this threat and use the park more often than others. Thus, understanding the health risks of heavy metals is critical to human physical health, although there are not many existing studies on the dangers of heavy metals in both rural and urban areas. The parameters are given in Table 1.

**Table 1.** Heavy metal’s uncertain concentrations in soils

Heavy metals	Probabilistic distribution	Parameters LN (mean, SD)
Cu	Logarithmic Normal	(39.97,16)
Cr		(115.04,26.43)
Ni		(37.34,5.39)
Zn		(144.73,51.57)
Pb		(42.59,23.46)
Cd		(0.29,0.14)
As		(8.31,2.21)
Hg		(0.21,0.20)
Mn		(694.4,95.17)
V		(86.42,11.28)

Meanwhile, in terms of health risk assessment, most of the past studies have generally focused on deterministic risk quantification of heavy metal in contaminated soils [18]. However, due to the possibility of underestimating or overestimating the risk levels due to the uncertainty of concentration and exposure parameters, it is basically impossible to accurately identify the most dangerous factors of risk with the point estimation method of deterministic parameters. While Monte Carlo simulation techniques can define risk above the guidance threshold and identify priority elements of risk assessment [18]. An example of a Monte Carlo simulated probabilistic risk estimation method to assess the health risk caused by mercury in soil will be presented below.

According to the HRA method recommended by USEPA, almost all exogenous compounds caused human health risks are divided into two categories, namely, non-carcinogenic risk (NCR) and carcinogenic risk (CR). Meanwhile, local people were divided into three groups, children, adult males and adult women. They were assessed separately according as their physiological differences. The Hazard index (HI) represents the cumulative NCR, and the total carcinogenic risk (TCR) is summation of the potential risk of all individual carcinogenic HMs. Estimated average daily intake (ADD) is divided into three categories based on the absorption route, which are intake, skin and inhalation. For carcinogenic risk, a CR value above the risk threshold ( $1 \times 10^{-4}$ ) indicates a significant cancer risk in humans, while below  $1 \times 10^{-6}$  is generally considered to cause little harm to human health. HRA uncertainty was minimized by Monte Carlo simulation, in consideration of the uncertainty of HM concentration and the variability of partial exposure factors. The concentration database of HMs was used to fit a log-normal distribution as an uncertain parameter and to simulate the optimal probability distribution of the exposure factors, which was finally included in the risk analysis.

#### 4. Limitations

Due to the different application of Monte Carlo simulation in different fields, it is not only difficult to describe the overall limitations, but also cannot guarantee that it will have a positive effect on the follow-up research in some fields. However, most of these practical applications cannot avoid using algorithms and code to achieve their ultimate research purpose. Therefore, this paper will focus on the algorithm and combine with specific fields to give the partial limitations of the Monte Carlo simulation. As mentioned in the introduction of SGMCMC, in the algorithm field, the large amount of time consumed by its repeated processing of the data and calculation of the parameters during the iteration limits the further application of MCMC [15]. Such problems with hardware and cost constraints also appear on the Monte Carlo search tree [20]. At the same time, if there is no enough and high quality of available data, the performance of the Monte Carlo algorithm will be unsatisfactory, which requires both the sampling method and the data itself [21]. Convergence analysis of asymptotic parameters relying on the approximate sampling distribution of Monte Carlo errors remains difficult when evaluating the reliability of the MCMC algorithm [22]. In more specific

applications such as the field of medical physics, fixed terms of model and code, the lack of data for adjusting the models, and the complexity of combining different disciplines in a single computational tool all limit the use of Monte Carlo simulations [23]. In the value-at-risk area, Monte Carlo simulations lack the ability to keenly capture the phenomena observed in financial data, such as time-varying fluctuations and long-term dependence [24].

## 5. Future Outlooks

In most cases, the research progress of Monte Carlo simulation not only belongs to Monte Carlo simulation itself, but also the breakthrough of the discipline it is applied to. As a popular research method or data processing method, future research should focus on the integration with other methods and fields. For instance, in the field of nuclear physics, the currents in the effective field theory (EFT) yield constructed new insights into the reactions of light and medium-mass nuclei, neutron matter, and electroweak atoms [24]. In the field of medical physics, emission tomography system is modified on Monte Carlo simulations of core-based imaging systems [25]. At the same time, the study of the Monte Carlo simulation algorithm itself should not be ignored. In addition to the issues to be addressed such as accurate sampling, the model adjustments and how to evaluate Monte Carlo algorithms, there are many future directions of Monte Carlo simulation. In terms of reducing computing time, with the progress of computer hardware, the very large number of lightweight Monte Carlo cores, known as "Monte Carlo groups", whose memory requirements are minimal, and the idea of remotely accessing data and counting using remote operations has achieved some results, but practical applications are still lacking [26, 27]. The improved Monte Carlo simulation still needs to be modified and adjusted repeatedly in practical application. How to make Monte Carlo simulation to adapt to different application environments to researchers may be a more important concern.

## 6. Conclusion

To sum up, this paper briefly introduces the three applications of Monte Carlo simulation in different fields and the related basic content. The Monte Carlo simulation from the Manhattan Project has evolved for a certain period, gradually spreading from nuclear physics to other disciplines such as engineering, finance and meteorology. It is sought after for its ability to break complex models into events and relationships between events and easily implement in computers. This then introduces new applications in three different areas. Although the way of verifying the results was not satisfactory, an adaptive long-term electricity price prediction model based on Monte Carlo simulation was designed. As a special Monte Carlo method, this paper introduces the basic framework of an extended class of SGMCMC (stochastic gradient Markov chain Monte Carlo) method based on the reduced computation time of subsampling. In the field of health risk assessment, the Monte Carlo simulation improves on the previous deterministic risk quantification, making the identification of risks more objective. Finally, this paper analyzes the limitations of the long computing time of Monte Carlo simulation, and proposes that the future development direction should be to solve the problem of Monte Carlo simulation itself while improving its adaptability in various fields.

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