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Note

On the Monte Carlo Simulation of Physical Systems

1. INTRODUCTION

Insofar as the modern powerful computers open new unique possibilities for application of the Monte Carlo method to the statistical simulation of the physical systems with many degrees of freedom [1–3], the role of the "quality" of pseudorandom numbers used in such simulations is becoming highly significant.

The first generator of pseudorandom numbers was initiated by Von Neuman, being based on successive calculation of the "middle-square" [4]. However, extensive studies carried out by Metropolis have shown that this generator is not good enough [5].

Interest to this old problem arose, when, making use of different generators of pseudorandom numbers, the results gave considerable disagreement [7, 8]; for example, this phenomenon was observed for the magnetization and renormalized coupling constant in the three-dimensional Ising model [7].

Obviously, there arise difficulties peculiar to the Monte Carlo method consisting in the need of (i) a good method of estimation of calculation error and (ii) finding a pseudorandom number generator that provides a speed of convergence as high as possible.

There exists a criterion via which one can estimate the calculation error as a function of the "quality" of pseudorandom numbers P_k. This is called the D_N discrepancy, being determined as follows [9].

Let Π^d be a unit hypercube in d-dimensional space: Π^d consists of all points P with Cartesian coordinates $0 \leqslant X_i \leqslant 1$ $(i = 1, ..., d)$; then

$$D_N(P_0, ..., P_{N-1}) = \sup_{P \in \Pi^d} |N \cdot X_1 \cdots X_d - S_N|, \tag{1}$$

where S_N is the number of points of the sequence $P_0, ..., P_{N-1}$, whose coordinates $(X_1^{(k)}, ..., X_d^{(k)})$, $k = 0, ..., S_N - 1$ satisfy inequality $0 \leqslant X_i^{(k)} \leqslant X_i$, $i = 1, ..., d$, $k = 0, ..., S_N - 1$. The geometrical meaning of the definition (1) is that $N \cdot X_1 \cdots X_d$ is the approximate number of points corresponding to a parallelepipied with a diagonal OP at ideal uniform distribution, while S_N is the number of points actually in this parallelepiped ($D_N \leqslant N$). Hence D_N estimates a maximal deviation of the real distribution of points from the ideal one.

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The following result is known [10]: if $f(P)$ is continuous together with its first partial derivatives, then

$$\left| \frac{1}{N} \sum_{K=0}^{N-1} f(P_k) - \int_{\Pi^d} f(P)\, dP \right| \leqslant C \cdot \frac{D_N}{N}, \tag{2}$$

where $C > 0$. In other words, good agreement between the empirical distribution function S_N of a pseudorandom sequence and a theoretical one gives a small integration remainder.

Therefore one must be able to generate pseudorandom sequence of points P_K in such a way, that D_N would grow as slowly as possible.

There exist also other "qualitative" characteristics of the P_K sequence, such as the χ^2 and ω^2 criteria, which do not, however, enable one to obtain estimates of the type (2).

If one is not interested in the dynamical origin of the pseudorandom sequence P_K, but considers it as a sequence of a random quantity ξ unfirformly distributed in a cube Π^d with a probability density $\rho(\xi) = 1$, then according to the central limit theorem the rate of convergence in (2) with high probability will be $1/\sqrt{N}$ [9]. Therefore, for ξ, $D_N \sim \sqrt{N}$.

Hence the rate of convergence depends on the dynamical origin of the pseudorandom sequence P_K and is determined by the rate of growth of D_N.

2. Pseudorandom Numbers as a Trajectory of Dynamical System

To explain why the behavior of D_N depends on the dynamical origin of P_K, let us discuss the P_K sequence as a trajectory of some dynamical system. For that, we assume the cube Π^d to be the phase space M of the dynamical system T, then

$$P_K = T \cdot T \cdot \cdots \cdot T \cdot P_0 \equiv T^K P_0, \tag{3}$$

where P_0 is the initial point of the trajectory. In such context the sequence of P_K points represents one of the trajectories of the dynamical system T. We will assume here that the phase volume of this dynamical system is conserved, i.e., the Liouville theorem holds.

Usually pseudorandom sequences are generated by the recursion relation [9–11]

$$X^{(K)} = F(X^{(1)}, \ldots, X^{(K-1)}), \tag{4}$$

where F is some function. For example, F may be taken in the form

$$X^{(K)} = F(X^{(K-1)}) = \{K \cdot X^{(K-1)}\}, \tag{5}$$

where $K \gg 1$ is a fixed integer number (under such a condition the Liouville theorem holds with, $T \equiv F$), and $\{\ \}$ denotes fractional part of the argument.[1]

As is known from the viewpoint of dynamical systems, the convergence of sums to the integral

$$\lim_{N\to\infty} \frac{1}{N} \sum_{K=0}^{N-1} f(T^K P_0) = \lim \frac{1}{N} \sum_{K=0}^{N-1} f(P_K) = \int_{\Pi^d} f(P)\, dP \tag{6}$$

is ensured if the dynamical system T is ergodic [12, 13]. Note that the rate of convergence may be arbitrary.

If we consider the pseudorandom number generator as a dynamical system, we can reformulate the statement (2); namely, the rate of convergence is provided by the dynamical properties of a system T:

$$\left| \frac{1}{N} \sum_{K=0}^{N-1} f(T^K P_0) - \int_{\Pi^d} f(P)\, dP \right| \leqslant C \cdot \frac{D_N(T)}{N}. \tag{7}$$

3. Statistical Properties of Dynamical Systems

A question arises regarding which property of the dynamical system T, given the pseudorandom number generator, ensures the slowest growth of discrepancy $D_N(T)$ and, thus, the high rate of convergence in (2). The principal argument is as follows:

It is known, that dynamical systems can be classified by the degree of growth of their statistical properties. These are systems with mixing, with n-fold mixing, and, finally, the Kolmogorov K-systems possessing maximally strong statistical properties [13]. All these dynamical systems are characterized by the property of relaxation [13, 16]. K-systems relax most rapidly because of their exponential instability [15].

Now it becomes clear that the slow growth of the deviation $D_N(T)$ will be provided if the dynamical system relaxes quickly to the equilibrium state. As we mentioned above, K-systems relax with exponential rate. For this reason K-systems are good candidates to be used as pseudorandom nubmer generators. We will characterize each pseudorandom number generator by its relaxation time τ, and if the time τ is less then the generator is better.

If from this viewpoint, we look at existing pseudorandom generators (5), then we see that they, also, are one-dimensional K-systems [13, 15, 18, 20]. The correlation function of this system behaves as ($K \gg 1$)

$$R_N = \frac{1}{12} \exp(-N \ln(K)), \tag{8}$$

[1] Its modifications were also used in [9, 11].

where

$$R_N = \frac{\int (X^{(M+N)} - \langle X^{(M+N)} \rangle)(X^{(M)} - \langle X^{(M)} \rangle)\, dX^{(M)}}{\int (X^{(M)} - \langle X^{(M)} \rangle)^2\, dX^{(M)}}$$

and

$$\langle X^{(M)} \rangle = \langle X^{(M+N)} \rangle = \tfrac{1}{2}; \tag{9}$$

i.e., K determines an essential characteristic of the time of correlation splitting

$$\tau_0 = 1/\ln(K). \tag{10}$$

Consider the set of points in a very small interval $\delta X^{(0)} \ll 1/K$. One can readily find the time τ, for which trajectories, coming from these points, almost uniformly fill the interval $[0, 1]$:

$$\tau = \tau_0 \cdot \ln\left(\frac{1}{\delta X^{(0)}}\right), \tag{11}$$

since $\delta X^{(N)} = K^N\, \delta X^{(0)} = \exp(N \ln(K))\, \delta X^{(0)}$. Physically, τ is an approximate time of the establishment of the stationary distribution function $\rho(X)$ to unity. The characteristic times in this system are coupled by the relation

$$\tau_0 < \tau. \tag{12}$$

From this discussion we see how growth of the deviation $D_N(T)$ of pseudo-random number generator, given by the dynamical system T, depends on statistical properties of T and is characterized by the relaxation time τ and it is better if system T is more unstable.

4. K-System Generators

If generator (5) is used to fill uniformly a d-dimensional cube, then the $X^{(1)}, ..., X^{(N)} ...$ sequence is formed, and "words" of d length are composed:

$$\begin{aligned} P_1 &= (X^{(1)}, ..., X^{(d)}), \\ P_2 &= (X^{(d+1)}, ..., X^{(2d)}), \\ &\cdots \end{aligned} \tag{13}$$

Here it is clear that instability, in d-dimensional cube, is again characterized by one-parameter K. Physically this means that instability of trajectories in Π^d in different directions has the same scale.

Is it possible that the instability of trajectories in $M = \Pi^d$ would be arbitrary in different directions? The answer is yes, if multidimensional K-systems are used. In

this paper we suggest using the automorphism of Π^d produced by the linear transformation

$$\begin{aligned} P_K &= AP_{K-1} \\ X_i^{(K)} &= \sum_{j=1}^{d} A_{ij} X_j^{(K-1)} \bmod 1, \end{aligned} \tag{14}$$

where $A = \|A_{ij}\|$ is an integer matrix with a determinant equal to one.[2] The last condition provides phase volume conservation. The dynamical system $T = \|A\|$ (14) is a K-system if and only if all eigenvalues of the matrix $A = \|A_{ij}\|$ are in modulus different from unity [12, 21–24].

The Sinai–Arov formula [19–24] allows us to calculate entropy of dynamical system (14), which is

$$h(T) = \sum_{|\lambda|>1} \ln |\lambda_k|, \tag{15}$$

as well as the upper estimate for the correlations splitting time,

$$\tau_0 \leqslant 1/h(T) = 1 \Big/ \sum_{|\lambda_K|>1} \ln |\lambda_K|, \tag{16}$$

and relaxation time,

$$\tau \leqslant \tau_0 \ln(1/\delta V_0^d). \tag{17}$$

The advantage of a pseudorandom number generator, given by a dynamical system (14), is that although the relaxation times τ (17) and (11) may be made equal, the "quality" of mixing in system (14) is higher owing to the fact, that in different directions the rate of instability is different and is proportional to the eigenvalues of the matrix A, which are quite arbitrary. Such "many-scale" mixing of directions ensures a slower growth of the discrepancy $D_N(T)$.

There exists one more argument in favor of the above state approach to the problem of convergence. When, say, lattice gauge theories are simulated [3] at the phase transition point, the gauge systems relax very slowly. Clearly, the role of a "thermostat" in this case is played by a dynamical system T, giving the pseudorandom number generator. Therefore, if the generator relaxation time is less compared to the characteristics times of the studies system, then it is better:

$$\tau_{\text{gener}} \ll \tau_{\text{CHAR}}(\beta); \qquad \beta = 1/KT. \tag{18}$$

In conclusion we note that we have failed to obtain an analytical estimate of D_N for generator (14). It is also unknown for the system (5). However, the viewpoint developed in this paper allows more purposeful searching for T systems, which will

[2] The inverse matrix $T^{-1} = A^{-1}$ is an integer too.

turn out to be more effective in Monte Carlo simulation, of essentially multi-dimensional problems.

As shown by numerical experiments (see next article), the pseudorandom sequences obtained with the use of (14) possess much better statistical characteristics than (5).

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