# Multicanonical Sampling of Rare Trajectories in Chaotic Dynamical Systems 

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#### Abstract

In chaotic dynamical systems, a number of rare trajectories with low level of chaoticity are embedded in chaotic sea, while extraordinary unstable trajectories can exist even in weakly chaotic regions. In this study, a quantitative method for searching these rare trajectories is developed; the method is based on multicanonical Monte Carlo and can estimate the probability of initial conditions that lead to trajectory fragments of a given level of chaoticity. The proposed method is successfully tested with four-dimensional coupled standard maps, where probabilities as small as $10^{-14}$ are estimated.


'Keywords: chaotic dynamical systems, rare trajectories, multicanonical Monte Carlo, coupled standard maps

## 1. Introduction

In chaotic dynamical systems, a number of rare trajectories with low level of chaoticity are embedded in chaotic sea, which show apparently small values of Lyapunov exponents. Also, there can be extraordinary unstable trajectories with apparently large values of Lyapunov exponent even in weakly chaotic systems.

Numerical search for such rare trajectories and quantitative estimation of their probabilities are important for the understanding of these dynamical systems. Even when Lyapunov exponent is converged to a unique value almost everywhere in a chaotic sea, the probability of finite-length trajectories of a given chaoticity reflects transient behavior of the system and hence provides information on fine structures in the state space 13].

In this paper, we develop a method for calculating probabilities of initial conditions that lead to trajectory fragments of a given level of chaoticity. This method is based on the multicanonical Monte Carlo algorithm [1], which is a version of dynamic Monte Carlo (Markov chain Monte Carlo) [3, 4] and provides a powerful tool -for calculating small probabilities under a given probability measure. The proposed method is tested with fourdimensional coupled standard maps. It is shown that the method can deal with rare events of very small probabilities such as $\sim 10^{-14}$.

The method proposed in this paper can be regarded as a variant of the method recently introduced in Yanagita and Iba [5]; the proposed method uses the multicanonical Monte Carlo instead of the replica exchange Monte Carlo used in [5]. A novelty in this paper is that probabilities of initial conditions that generate rare trajectories

[^0]are successfully estimated, while no quantitative result is obtained in the previous paper [5]. Also, the multicanonical algorithm has advantages over the replica exchange Monte Carlo; it enables direct computation of the desired probabilities and is efficient in cases with first order transitions [1].

Our studies are partly motivated by the studies 6], where rare structures with high or low chaoticity are explored by simulating fictitious particles that are moved, split, and systematically erased; their method can be regarded as tracking rare "pseudo-orbits" in a parallel manner. The method proposed in this paper samples initial conditions and seems complementary to their approach. There are also references [7, 9, 10, 11] that discuss sampling of unstable periodic orbits in chaotic systems by dynamic Monte Carlo or related methods. None of these studies, however, seems to compute probabilities of rare trajectory fragments using the multicanonical algorithm.

## 2. Algorithm

### 2.1. Forgetting Time as a Measure of Chaoticity

Let us consider a deterministic dynamical system $x(t+1)=\psi(x(t))$ with discrete time $t=1,2, \ldots$ and assume a trajectory $x(t)$ originated from an initial condition $x(0)=x_{0}$. Specify a measure $f$ for the chaoticity of the trajectory $x(t)$ and consider it as an integer-valued function $f\left(x_{0}\right)$ of the initial condition $x_{0}$; for a real-valued $f$, appropriate discretization of its value is assumed. Then, our interest is in estimating the probability

$$
P(\tilde{f})=\frac{1}{D} \int \delta\left(f\left(x_{0}\right)-\tilde{f}\right) d x_{0}
$$

where $\delta$ is defined as $\delta(s)=1$ if $s=0 ; \delta(s)=0$ otherwise. $d x_{0}$ is uniform measure on the space of initial conditions and $D$ is the volume of the entire space.

An important point is the choice of $f\left(x_{0}\right)$; assuming finite precision arithmetic of computers, it should be something like "approximate Lyapunov exponent" of a finite piece of the trajectory starting from $x_{0}$.

A possible way is to fix the length $T$ of the trajectories and define $f\left(x_{0}\right)$ as the largest eigenvalue $\lambda_{T}\left(x_{0}\right)$ of the product $\prod_{t=1}^{T} \mathbf{J}(x(t))$ of the Jacobian matrices $\mathbf{J}(x(t))$ along the piece of the trajectory $x(t)$ starting from $x_{0}$. Here $(i, j)$-component of $\mathbf{J}(x(t))$ is given by $\mathbf{J}_{i j}(x(t))=$ $\left.\frac{\partial \psi_{i}(x)}{\partial x_{j}}\right|_{x=x(t)}$, where $\psi_{i}$ and $x_{i}$ are $i$ th component of the function $\psi$ and its argument, respectively. This way of choosing $f\left(x_{0}\right)$ is, however, not suited for numerical computation when $\lambda_{T}\left(x_{0}\right)$ is strongly dependent on $x_{0}$. When $\lambda_{T}\left(x_{0}\right)$ is large we should choose small $T$ to control the effect of round-off error. On the other hand, larger $T$ is desirable in the region of small $\lambda_{T}\left(x_{0}\right)$ to filter out trajectories with low chaoticity. Thus, it is difficult to choose the value of $T$ adequate for all values of $\lambda_{T}\left(x_{0}\right)$.

Our solution is to reverse the idea and use the minimum value $T_{\epsilon}\left(x_{0}\right)$ of $T$ that satisfies $\lambda_{T}\left(x_{0}\right) \epsilon>1$ as a measure of chaoticity, where $\epsilon$ is a small constant beyond the machine epsilon; larger value of $T_{\epsilon}\left(x_{0}\right)$ means larger number of time-steps required to forget the initial condition and implies lower chaoticity. The switching from $f\left(x_{0}\right)=\lambda_{T}\left(x_{0}\right)$ to "forgetting time" $f\left(x_{0}\right)=T_{\epsilon}\left(x_{0}\right)$ provides a computationally stable criterion of chaoticity, because by definition the latter is insensitive to round-off error.

### 2.2. Multicanonical Algorithm

We introduce the multicanonical algorithm to estimate the probability $P(f)$; the algorithm consists of two stages, training and measurement. In the training phase, we construct the approximate probability $\tilde{P}(f)$ step-by-step through dynamic Monte Carlo simulations. At each step, we perform Monte Carlo simulation with the weight function $1 / \tilde{P}\left(f\left(x_{0}\right)\right)$ using the current estimate of $\tilde{P}(f)$. If $\tilde{P}(f)$ is a good approximation to $P(f)$ in a prescribed interval of $f$, the histogram $h(f)$ is almost flat in the interval, because

$$
h(f) \propto \frac{1}{D} \int \delta\left(f\left(x_{0}\right)-f\right) \frac{1}{\tilde{P}\left(f\left(x_{0}\right)\right)} d x_{0}=\frac{P(f)}{\tilde{P}(f)} \simeq 1
$$

If $h(f)$ is not sufficiently flat, we modify $\tilde{P}(f)$ until an almost flat histogram of $f$ is obtained. Several methods are proposed for efficient tuning of the weight in the training phase; in this study, we use a method due to Wang and Landau 12]. After we obtain a good approximation of $P(f)$ we enter the measurement phase and perform a long run of simulation with a fixed weight $1 / \tilde{P}\left(f\left(x_{0}\right)\right)$. Then, the final estimate $P^{*}(f)$ of $P(f)$ is obtained as $P^{*}(f) \propto$ $h(f) \tilde{P}(f)$.

The key to the implementation of the algorithm is that the weight $1 / \tilde{P}\left(f\left(x_{0}\right)\right)$ of $x_{0}$ is expressed with a composite function of a univariate function $\tilde{P}(f)$ and a known
function $f\left(x_{0}\right)$; it enables easy adaptation of the weight using outputs of the simulations. On the other hand, the multicanonical algorithm enjoys fast mixing of the Markov chain; sampling in a wide range of $f$ realizes a kind of "annealing" effect and the convergence becomes much better compared with the cases where only the tail regions are sampled.

So far we discuss the generic algorithm. To implement the multicanonical algorithm in the present case, where $f\left(x_{0}\right)=T_{\epsilon}\left(x_{0}\right)$, we should specify dynamic Monte Carlo algorithm for the sampling with the weight $1 / \tilde{P}\left(T_{\epsilon}\left(x_{0}\right)\right)$. Here we use the Metropolis algorithm [3, 4], in which a candidate $x_{0}^{\text {new }}$ is generated using a hierarchical proposal distribution used in [5]. The candidate $x_{0}^{\text {new }}$ is accepted if and only if a uniform random number $r \in[0,1)$ satisfies $r<\frac{\tilde{P}\left(T_{\epsilon}\left(x_{0}^{\text {old }}\right)\right)}{\tilde{P}\left(T_{\epsilon}\left(x_{0}^{\text {new }}\right)\right)}$, where $x_{0}^{\text {old }}$ is the current value of $x_{0}$; to compute $T_{\epsilon}\left(x_{0}^{\text {new }}\right)$ at each step of the Metropolis algorithm, we simulate the trajectory from the initial condition $x_{0}^{\text {new }}$ until $\lambda_{T}\left(x_{0}^{n e w}\right) \epsilon>1$.

### 2.3. Computation of the Largest Eigenvalue

To implement the proposed algorithm for highdimensional dynamical systems, we should compute the largest eigenvalue $\lambda$ of the matrix $\mathbf{J}_{T}=\prod_{t=1}^{T} \mathbf{J}(x(t))$ efficiently. In this study, we approximate it using the power method as $\lambda \simeq\left\|\mathbf{J}_{T}^{m} \xi\right\|$, where $\xi$ is a constant vector of unit length $\|\xi\|=1$. We found that $m=1$ often gives a good approximation.

## 3. Numerical Experiments

### 3.1. Searching Low Chaoticity

Let us consider four-dimensional coupled standard maps

$$
\begin{align*}
u_{n+1} & =u_{n}-\frac{K}{2 \pi} \sin \left(2 \pi v_{n}\right)+\frac{b}{2 \pi} \sin \left(2 \pi\left(v_{n}+y_{n}\right)\right) \\
v_{n+1} & =v_{n}+u_{n+1}  \tag{1}\\
x_{n+1} & =x_{n}-\frac{K}{2 \pi} \sin \left(2 \pi y_{n}\right)+\frac{b}{2 \pi} \sin \left(2 \pi\left(v_{n}+y_{n}\right)\right), \\
y_{n+1} & =y_{n}+x_{n+1}
\end{align*}
$$

which is a well-studied example of volume preserving maps.

First, we test the efficiency of the proposed algorithm to find tiny tori in chaotic sea. In Fig. 11 a pair of tori in chaos found by the algorithm is plotted on the $\left(u_{n}, v_{n}\right)$ plane; values of parameters $K=7.8$ and $b=0.001$ are chosen that most of the state space is covered by a chaotic sea. The threshold $\epsilon$ is $2^{-43}$. The values of $T_{\epsilon}$ corresponding to the initial conditions that lead to these tori are larger than 199 and the probabilities $P\left(T_{\epsilon}\right)$ are as small as $10^{-12}$. The number of initial conditions tested in the proposed method is about $4 \times 10^{9}$.


Figure 1: A pair of tiny tori in a chaotic sea found by the proposed method. Projections on the $\left(u_{n}, v_{n}\right)$-plane are shown. Enlargement of a tiny area in the small circle in the left panel is given in the right panel; further enlargement is given in the lower panel. $K=7.8$ and $b=0.001$.

### 3.2. Probabilities $P\left(T_{\epsilon}\right)$

An advantage of the multicanonical algorithm is that it computes probabilities $P\left(T_{\epsilon}\right)$ of $T_{\epsilon}$ under uniform sampling of initial conditions. The probability of trajectory fragments that stays long time near tiny tori and/or cantori will reflect fine structures of phase space, which can be quantified by $P\left(T_{\epsilon}\right)$. In Fig. 2, $P\left(T_{\epsilon}\right)$ for the model (1) is plotted. The result indicates that, in this parameter range, the volume of small regular regions decrease under increasing $K$, while increase under increasing $b$.

The number of initial conditions tested in the proposed algorithm is $3 \times 10^{9} \sim 3 \times 10^{10}$ for each curve including training phase and rejected candidates; the corresponding computational times are $17 \sim 125$ hours using a single core of Intel Xeon X5365, which is a quad-core CPU. These results show that the proposed method can compute probabilities down to $\sim 10^{-14}$ within reasonable computational times.

For the comparisons, results of naive random sampling are also shown in Fig. 2 For $(K, b)=(6.0,0.1)$, there is an overall agreement of the outputs following from the two sampling approaches. For $(K, b)=(7.8,0.1)$, both results are also consistent, but naive random sampling with comparable computational efforts $\left(1.4 \times 10^{10}\right.$ initial configurations) gives meaningful results only in a high probability region, as seen in the upper panel of Fig. 2.

In these examples, we set the number $m$ of iteration defined in Sec. 2.3 to unity; $m=2$ and 3 are also tested and slight differences are found in some cases.

## 4. Summary and Discussion

A quantitative method based on multicanonical Monte Carlo is proposed for searching rare trajectories in chaos. The proposed method is tested with four-dimensional coupled standard maps and successfully computes the probability of the forgetting time $T_{\epsilon}$ down to $\sim 10^{-14}$.

Applications of the proposed method to dissipative and/or multi-basin systems will be interesting, as well as search for highly unstable trajectories in weakly chaotic systems. Another interesting subject is to develop a way to relate $P\left(T_{\epsilon}\right)$ to "escape rate" and hence interpret it in the thermodynamic formalism [13], which connects our approach to existing studies on large deviations in chaos.


Figure 2: The probability $P\left(T_{\epsilon}\right)$ is plotted as a function of $K$ (upper panel, $b=0.1$ ) and $b$ (lower panel, $K=7.8$ ), where $\epsilon=2^{-43}$. The results of naive random sampling are shown by the symbol + , only when more than 10 samples are available. The symbols • at the right edge of the plot indicate values of the probability $P\left(T_{\epsilon} \geq 200\right)$.

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