Exploration of order in chaos using the replica exchange Monte Carlo method

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Abstract. A method for exploring unstable structures generated by non-linear dynamical systems is introduced. It is based on the sampling of initial conditions and parameters using the replica exchange Monte Carlo method, and it is efficient in searching for rare initial conditions and in the combined search for rare initial conditions and parameters. Examples discussed here include the sampling of unstable periodic orbits in chaos and searching for the stable manifold of unstable fixed points, as well as construction of the global bifurcation diagram of a map.

Keywords: classical Monte Carlo simulations, stochastic search, nonlinear dynamics

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1. Introduction

Non-linear dynamical systems exhibit very complex structures in the phase space [1, 2]. There can be a number of stable or unstable fixed points, periodic orbits, chaotic saddles, and more intricate invariant manifolds. Basin structures corresponding to these invariant manifolds can also be very complicated. The investigation of these structures is an important subject in the study of dynamical systems.

It is, however, not easy to capture these global structures through time evolution from randomly chosen initial conditions because they are often unstable and correspond to very rare initial conditions. The analysis of these structures requires an efficient algorithm for sampling rare trajectories from rare initial conditions, which acts as a tool for analyzing non-linear dynamical systems. Moreover, the properties of chaotic or multibasin dynamical systems are often sensitive to the choice of values of the parameters. Then, an additional complexity arises when we do not have precise knowledge about the values of parameters for which interesting structures appear. An algorithm using which we can perform combined searches of the space of initial conditions and of the parameter space is required for analyzing dynamical systems.

In this paper, we introduce a method based on the Markov chain Monte Carlo method (MCMC) [3–5], which is efficient in the search for rare initial conditions and in the combined search among rare initial conditions and parameters. In the proposed algorithm, we identify the initial conditions of trajectories as microscopic states to be sampled, and we assign each of them an artificial ‘energy’ that represents a measure of the ‘atypicality’ of the trajectory starting from the initial condition. These initial conditions are sampled
Exploration of order in chaos using the replica exchange Monte Carlo method by MCMC, and a set of atypical trajectories is obtained. This approach is easily extended to the combined searching of the space of initial conditions and of the parameter space. An essential concept here is the use of the direct product of the initial conditions and parameters as a state space explored by MCMC.

In both cases, however, naive applications of MCMC will be impaired by the sensitive dependence on initial conditions and parameters in non-linear dynamical systems, which would lead to a highly multimodal energy function. Here, we use the replica exchange Monte Carlo method (REM), which is also known as parallel tempering (PT), to circumvent the difficulty. REM is useful for sampling on a rugged energy surface and has been used extensively for finite-temperature simulation of spin glass [6,7] and biomolecules [8,7]. When we generate multiple samples using conventional optimization methods such as simulated annealing, it is difficult to control the probability of the repeated appearance of the same (or similar) items in the set of samples obtained. The advantage of REM is that it realizes unbiased sampling from the given ensemble even in the region corresponding to low ‘temperatures’.

The idea of using MCMC or a related algorithm for sampling rare trajectories in non-linear dynamical systems has already been reported [9]–[15], although a combined search for initial conditions and parameters has rarely been studied.

These studies can be classified into two categories. Some of them [9]–[13], including an earlier work [9] and recent studies [13,12], involved frameworks where the states to be sampled by the algorithm are entire trajectories or orbits, instead of initial conditions of the trajectories. ‘Transition path sampling’ [16,10,11,17], used mostly for sampling trajectories between two metastable states, is also based on a similar choice of state space, that is, a state consists of the array of positions (and momenta) of particles at all time steps in a trajectory. The algorithm proposed in this paper is quite simplified in comparison, with the choice of initial condition as a state variable. It is also a natural choice for a deterministic, but not necessarily reversible, dynamical system. In the following sections, we will show that the proposed algorithm can deal with various kinds of problems suitably.

Another type of algorithm [14,15] approximates ‘pseudo-trajectories’ with the desired property by a set of particles, each of which obeys the original equation of motion. Using a genetic algorithm such as the split/delete procedure, efficient sampling of rare trajectories is realized. This approach is a type of sequential Monte Carlo [18,19] or diffusion Monte Carlo [20,19] approach, but not genuine MCMC. It can also be interpreted as a multiparticle version of an ingenious ‘staggered-step’ algorithm [21] developed earlier. The approach appears effective for trajectories with positive Lyapunov numbers; however, its advantage might be reduced in a search for trajectories with negative Lyapunov numbers, where split trajectories do not diverge rapidly without strong external noise. Nonetheless, it appears to capture different aspects of chaotic systems and will be complementary to the method proposed in this paper.

This paper is organized as follows. In section 2, we explain the concept of the proposed method. In section 3, two examples of initial condition sampling are discussed. The first one is a toy example that entails sampling of the unstable periodic orbits of the Lorenz model. The second one entails sampling of the stable manifold of the unstable fixed points of a double pendulum with dissipation, which is a much more difficult and interesting example. In section 4, the searching of the parameter space and combined searching of the parameter space and initial condition space using a modified algorithm...
are studied. Section 5 presents the discussion of the numerical results and describes further work.

2. Method

2.1. State vector

In the basic algorithm for discrete-time dynamics with a given set of parameters, the initial condition $X = (x_1, \ldots, x_n) \in \mathbb{R}^n$ of a trajectory is used as a state variable that characterizes the trajectory evolving from the initial condition. In a continuous-time case, it is often better to include the time $T$ when desired phenomena occur; then, a state will be $X = (x_1, \ldots, x_n, T) \in \mathbb{R}^{n+1}$. Finally, when the parameters are also unknown, the state vector will be $X = (x_1, \ldots, x_n, T, \alpha_1, \ldots, \alpha_m) \in \mathbb{R}^{n+1+m}$, where $\alpha = (\alpha_1, \ldots, \alpha_m)$ is a vector of unknown parameters.

2.2. Energy function and Gibbs distribution

In order to explore rare structures in the phase space, we should construct a fictitious ‘energy’ function $E(X)$ defined on the state space. The function depends on the type of rare orbit that we want to explore. For the detection of periodic orbits of a map $x_{n+1} = f(x_n)$, a simply possibility for the energy function is $E(x_0) = \log(|f^n(x_0) - f(x_0)|)$, where the state $X$ coincides with the initial condition $x_0$ of the iteration. The other choices of energy functions that can be used to explore an atypical structure in the phase space are shown in section 4, where $E$ may also depend on $T$ and $\alpha$.

Once we define the energy function, it is straightforward to define the Gibbs distribution with the energy

$$p(X) = \frac{\exp(-\beta E(X))}{Z(\beta)}, \quad Z = \int \exp(-\beta E(X)) \, dX. \quad (1)$$

While $p(X)$ coincides with the uniform density in a prescribed region when $\beta$ takes a small value, it concentrates to regions with small values of $E$ when $\beta$ increases, and we can then collect samples of trajectories (and parameters) of desired properties.

2.3. Metropolis algorithm

Now, the problem of sampling atypical trajectories is reduced to that of sampling from the density $p(X)$. Here, we use the Metropolis algorithm [22], the simplest implementation of the MCMC concept. The Metropolis algorithm used here is essentially the same as the standard one commonly used in statistical physics. There is, however, an important difference in the actual implementation, that is, we should simulate the trajectories of the length $T$ from the initial condition $x$ with the parameter $\alpha$ at each trial of changing $x$, $T$, and $\alpha$. If we explicitly represent this difference, the iteration of the algorithm is described as follows:

(i) Draw a perturbation to current states $(\Delta x, \Delta T, \Delta \alpha)$ from a prescribed ‘trial’ density $q$, which defines a move set. Hereafter, the mirror symmetry

$$q(-\Delta x, -\Delta T, -\Delta \alpha) = q(\Delta x, \Delta T, \Delta \alpha)$$
of the density \( q \) is assumed. Then, when the current values of \((x, T, \alpha)\) are \((x^{(n)}, T^{(n)}, \alpha^{(n)})\), the candidate next state is defined as \((x', T', \alpha') = (x^{(n)} + \Delta x, T^{(n)} + \Delta T, \alpha^{(n)} + \Delta \alpha)\).

(ii) Run the simulation of length \( T' \) of the dynamical system with parameter \( \alpha' \) from the initial condition \( x' \). From the result, \( E(\alpha', T', x') \) is computed.

(iii) Draw a uniform random number \( R \in [0, 1] \). If and only if

\[
R < \frac{\exp(-\beta E(x', T', \alpha'))}{\exp(-\beta E(x^{(n)}, T^{(n)}, \alpha^{(n)}))},
\]

the new proposal is accepted: \( x^{(n+1)} = x' \), \( T^{(n+1)} = T' \), \( \alpha^{(n+1)} = \alpha' \); otherwise nothing is changed: \( x^{(n+1)} = x^{(n)} \), \( T^{(n+1)} = T^{(n)} \), \( \alpha^{(n+1)} = \alpha^{(n)} \).

(iv) Return to step (i).

An important issue in treating unstable structures in potentially chaotic systems is the choice of density \( q \), or, equivalently, the set of moves. The point is that the moves should be hierarchical for efficient sampling, that is, the coexistence of tiny and large changes in phase space is essential [21]. Here we adopt the method introduced in [21], that is, the element \( \Delta x_i \) of the perturbation \( \Delta x \) takes a value \( s \times d \times 10^{-e} \), where \( d \) and \( e \) are random integers uniformly distributed in \( d \in [1, 9] \) and \( e \in [N_{e, \min}, N_{e, \max}] \), and \( s \) is a binary random number that takes the values \( \pm 1 \) with probability 0.5. The parameters \( N_{e, \min} \) and \( N_{e, \max} \) of the algorithm define the logarithmic scales of the largest and smallest perturbations, respectively. The corresponding trial density \( q(x_i) \) becomes a mixture of uniform distributions with different scales. It has a sharp peak near zero, as well as very long tails. The components of \( \Delta \alpha \) and \( \Delta T \) are also generated in a similar manner. The results presented in sections 3 and 4 do not significantly depend on the parameters \( N_{e, \min} \) and \( N_{e, \max} \).

If the desired atypical trajectories are unstable, numerical errors at large \( T \) accumulate because of the unstable nature of the trajectories. This phenomenon may lead to a tendency for the frequency of the unstable trajectory to become smaller. This effect can be checked by quantitative comparison of the results with different \( T \) and different numerical precisions, which we have left for future studies.

This version of the Metropolis algorithm appears to provide a simple and universal means of treating the Gibbs distribution (1). However, the efficiency of the algorithm may decrease when \( \beta \) increases, as in the case of a highly multimodal energy function. This problem can be solved by means of the REM algorithm described in section 2.4.

### 2.4. The replica exchange Monte Carlo method

REM provides an efficient way to investigate systems with rugged free-energy landscapes [23, 24, 7], particularly at low temperatures. In the present context, it has been used for sampling of unstable orbits [12, 13]. REM can also be useful in the framework of ‘transition path sampling’ [11, 17].

In a REM simulation, a number of systems \( \{X_{(m)}\} \) with different inverse temperatures \( \beta_m \) (replicas) are simulated in parallel. At regular intervals, an attempt is made to exchange the configurations of selected, usually adjacent, pairs of replicas. It is accepted with the probability

\[
P(X_{(m+1)} \leftrightarrow X_{(m)}) = \min[1, \exp(\Delta \beta \Delta E)],
\]

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where \( \Delta \beta = \beta_{m+1} - \beta_m \) is the difference between the inverse temperature of the two replicas and \( \Delta E = E(X_{(m+1)}) - E(X_{(m)}) \) is the energy difference between them.

The exchange of replicas with different temperatures effectively reproduces repeated heating and annealing, which avoids trapping in local minima of the energy. Note that it is especially useful with the hierarchical moves defined in the section 2.3, because large moves are accepted at high temperatures and tiny moves dominate at low temperatures.

On the other hand, the rule of stochastic exchange described above preserves the joint probability distribution
\[
\prod_m P_{\beta_m}(X_{(m)}),
\]
as shown in the literature, e.g., [24]. Thus, even with the annealing effect, the probability distribution of each replica \( X_{(m)} \) coincides with \( P_{\beta_m}(X_{(m)}) \), which implies that an unbiased set of samples is obtained at all inverse temperatures \( \{\beta_m\} \).

3. Initial condition sampling

In this section, we show examples of initial state sampling using our proposed method. One example is the search for unstable periodic orbits (UPOs) of the Lorenz model. Another interesting example is sampling of rare orbits in a double-pendulum system, where initial conditions that locate on the stable manifold of unstable fixed points are sampled using our proposed method.

3.1. Unstable periodic orbits of the Lorenz model

In this section, we show that unstable periodic orbits (UPOs) in a continuous-time dynamical system can be detected using our proposed method. UPOs are considered to be important objects that govern the properties of chaos [2], and many studies have dealt with the computation of UPOs [25]–[28], [12,13]. Here, we show how the proposed method works with a familiar example instead of proving that our method is superior to all of these existing methods. It is, however, useful to note that our method with REM can generate UPOs uniformly under the assumption of uniform measure in the space of initial conditions. This fact suggests that it can be useful in the global searching for UPOs in combination with other methods.

Here, we consider the Lorenz equations [29,30]
\[
\begin{align*}
\dot{x} &= \sigma(y - x), \\
\dot{y} &= rx - y - xz, \\
\dot{z} &= xy - bz,
\end{align*}
\]
as a typical continuous-time chaotic system, where \( \sigma, r \) and \( b \) are parameters of the system. The state of the system is denoted in a vector format as \( \vec{x} = (x, y, z) \), and the initial condition is written as \( \vec{x}_0 = (x_0, y_0, z_0) \). The flow generated by the dynamical system (2) is expressed as \( \varphi^t \), and the orbit determined by the initial condition \( \vec{x}_0 \) is written as \( \vec{x}_t = \varphi^t(\vec{x}_0) \).

The state sampled by REM is defined by \( X \equiv (\vec{x}_0, T) = (x_0, y_0, z_0, T) \). Then, a candidate energy function is given as
\[
E(\vec{x}_0, T) = \log(|\varphi^T(\vec{x}_0) - \vec{x}_0| + \epsilon).
\]
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The parameter $\epsilon \ll 1$ is a constant for avoiding divergence of the energy. When the orbit $\{\varphi'(\vec{x}_0); t \in \mathbb{R}\}$ is periodic, there exists a time $T$ such that $\varphi^T(\vec{x}_0) = \vec{x}_0$, and the energy of the initial condition $\vec{x}_0$ takes the minimum value $\log(\epsilon)$.

There are, however, problems with the naive choice of the energy function (3). First, the energy $E(\vec{x}_0, 0)$ always takes the minimum value, because $\varphi^0(\vec{x}) = \vec{x}$. In addition, when an initial state $\vec{x}_0$ locates on a fixed point, the energy of the initial state takes the minimum value for all $T$. This fact implies that almost all initial conditions sampled by the energy function will be in the vicinity of fixed points. To avoid these unfavorable situations, we will add a penalty term $P(\vec{x}_0, T)$ to the naive energy function (3). An improved energy function is

$$E(\vec{x}_0, T) = \log(|\varphi^T(\vec{x}_0) - \vec{x}_0| + P(\vec{x}_0, T) + \epsilon), \quad (4)$$

$$P(\vec{x}_0, T) = g\left(\frac{1}{T} \int_0^T \varphi^T(\vec{x}_0)^2 \, \mathrm{d}\tau, v_c\right) + g(T, T_c), \quad (5)$$

where we use an auxiliary function $g(s, s_c) = \Theta(s_c - s)((1/s) - (1/s_c))$. $\Theta(s)$ is the Heaviside function defined by $\Theta(s) = 1$ if $s \geq 0$; otherwise $\Theta(s) = 0$. The first term in equation (5) represents a penalty for slower ‘average speed’ of the trajectory, where $v_c$ is a threshold parameter. When an initial condition is in the vicinity of a stable or unstable fixed point, the orbit stays near the point for a certain time. Then, the averaged speed decreases and the value of the integral in the penalty term increases, which causes a large energy value. The second term is a penalty for the states that have small $T$, where $T_c$ is a threshold parameter.

For the sampling of the initial condition $\vec{x}_0$ of the Lorenz model, we consider the symmetry $(x, y) \leftrightarrow (-x, -y)$ of the equations. We sample initial conditions from the Poincaré section $\vec{x}_0 = (x_0, y_0, r - 1)$, where $x_0 \in [0, 20]$ and $y_0 \in [0, 20]$. The period $T$ of orbits is assumed to be in the interval $[0, T_{\text{max}}]$, where $T_{\text{max}} = 6.0$. Using the energy function (4), the states $X = (\vec{x}_0, T)$ are sampled by the proposed method. Thirty-one replicas with $\beta = 2.0 + 0.1i$, $i = 0, 1, \ldots, 30$, are used.

The samples obtained using our proposed method are plotted on the $(E, T)$ plane in figure 1(a) for different temperatures, which are obtained in parallel in a REM calculation. For lower temperatures, the energy takes smaller values for specific values of the period $T$, which correspond to UPOs.

In figure 1(b), the initial condition samples with $E(\vec{x}_0, T) \leq -1.5$ are plotted on the Poincaré section. The initial conditions form clusters, and each cluster corresponds to the initial condition in the vicinity of a different UPO. In each cluster, we select the initial condition that has the minimum energy and calculate orbit $\varphi^T(\vec{x}_0)$ starting from the initial condition. Typical orbits are shown in figure 2. These orbits are closed with high precision, i.e., the difference between $\vec{x}_0$ and $\varphi^T(\vec{x}_0)$ is of the order of $10^{-3}$, thereby indicating that they are UPOs.

We tested these orbits using AUTO software [31]. An orbit detected using our algorithm is used as an initial guess for Newton’s method implemented in AUTO. We observe that the convergence is remarkably quick, which indicates that the iteration begins ‘sufficiently near’ the UPOs. The difference between the output of Newton’s method and the initial guess is also very small.
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Figure 1. (a) Samples generated using our proposed method are plotted on the \((E, T)\) plane. The crosses, triangles, filled circles, and circles correspond to \(\beta = 2, 3, 4, 5\), respectively. (b) Samples with the energy lower than \(-1.5\) are plotted on the Poincaré section \((x, y, r - 1)\). The clusters, each of which corresponds to different minima, are identified by using cluster analysis and they are plotted using different symbols. 25 clusters are shown. The inset is a magnification. \(\epsilon = 10^{-3}, T_c = 4, v_c = 4, N_{\text{e}}^{\text{min}} = 1\), and \(N_{\text{e}}^{\text{max}} = 5\).

3.2. The stable manifold of unstable fixed points of a double pendulum

Let us consider the following dynamics of the double pendulum with dissipation:

\[
\ddot{\theta}_1 = \frac{\sin(2(\theta_1 - \theta_2)) \dot{\theta}_1^2 + 2 \sin(\theta_1 - \theta_2) \dot{\theta}_2^2 + 3 \sin(\theta_1) + \sin(\theta_1 - 2\theta_2)}{\cos(2(\theta_1 - \theta_2)) - 3} - k\dot{\theta}_1, \\
\ddot{\theta}_2 = -\frac{2 \sin(\theta_1 - \theta_2) \left(2\dot{\theta}_1^2 + \cos(\theta_1 - \theta_2) \dot{\theta}_2^2 + 2 \cos(\theta_1)\right)}{\cos(2(\theta_1 - \theta_2)) - 3} - k\dot{\theta}_2,
\]

(6)

where \(k\) is a damping coefficient.

The double-pendulum system (6) has three unstable fixed points: \((\theta_1, \dot{\theta}_1, \dot{\theta}_2, \dot{\theta}_2) = (\pi, 0, 0, 0), (\pi, 0, \pi, 0)\), and \((0, \pi, \pi, 0)\). Each unstable fixed point corresponds to an ‘inverted’ state of the pendulums. Starting from any initial condition \(\vec{x}_0 = (\theta_1, \dot{\theta}_1, \theta_2, \dot{\theta}_2) = (0, \omega_1, 0, \omega_2)\), however, almost all trajectories converge to the stable fixed point \((\theta_1, \dot{\theta}_1, \dot{\theta}_2, \dot{\theta}_2) = (0, 0, 0, 0)\) by dissipation originating from the friction at the hinge.

In this system, we attempt to detect atypical trajectories that converge to unstable fixed points. When an initial condition locates on the stable manifold of an unstable fixed point, the orbit starting from such an initial condition converges to the unstable fixed point after a long time evolution. We search for such an atypical initial state on the Poincaré section \((\theta_1, \dot{\theta}_1, \dot{\theta}_2, \dot{\theta}_2) = (0, \omega_1, 0, \omega_2)\).

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Figure 2. Typical unstable periodic orbits of the Lorenz model sampled by REM are shown. Each orbit is produced from time evolution starting from the initial condition that has the minimum energy in a cluster shown in figure 1(b).

The state sampled using our method is set as $X = (\omega_1, \omega_2, T)$. Many energy functions are possible. Here, we attempt to find trajectories that converge on one of the three fixed points and choose the energy as

$$E(\omega_1, \omega_2, T) = \log(E_k(\omega_1, \omega_2, T) + E_p(\omega_1, \omega_2, T)),$$

$$E_k(\omega_1, \omega_2, T) = |\dot{\theta}_1(T)| + |\dot{\theta}_2(T)|,$$

$$E_p(\omega_1, \omega_2, T) = \min[\cos(\theta_1(T)) \cos(\theta_2(T)), \cos(\theta_1(T)) + \cos(\theta_2(T))] + 1,$$

where $E_k$ represents the ‘kinetic energy’ of the pendulum at time $T$ starting from an initial condition defined by $(\omega_1, \omega_2)$. The term $E_p$ represents an artificial ‘potential energy,’ which has minima at each of the three unstable fixed points. Note that if we want to find trajectories that converge to a given unstable fixed point, we can use other artificial potential energies such as $E_p'(\omega_0, \omega_1, T) = |\theta_1(T) - \pi| + |\theta_2(T) - \pi|$. The energy landscape defined by (7) is shown in figure 3(a), where the energy $E(\omega_1, \omega_2, T)$ versus $\omega_1$ and $\omega_2$ is plotted for a fixed time, $T = 5$. A rugged structure is clearly observed and the sampling efficiency is expected to increase when REM is used.

We next discuss the result of a simulation with 51 replicas with $\beta_i = 2.0 + 0.2i$ for $i = 0, 1, \ldots, 30$. In figure 3(b), the initial states sampled using our method are plotted.
Figure 3. (a) Rugged energy landscape $E(x_0, T)$ with fixed $T = 5.0$ as a function of $\omega_1$ and $\omega_2$. (b) Samples are plotted on the $(E, \omega_1)$ plane for different temperatures; $\beta = 0.1, 1.1, 2.1, 3.1, 4.1, 5.1$. The sampling is performed using 51 replicas with $\beta = 0.1i$ for $i = 1, 2, \ldots, 51$. $\epsilon = 10^{-5}, N_{\text{min}}^e = 1$, and $N_{\text{max}}^e = 9$.

on the $(\omega_1, E)$ plane for replicas with inverse temperatures $\beta = 0.1, 1.1, 2.1, 3.1, 4.1, 5.1$. The points are scattered at higher temperatures, but they are concentrated in separate regions when the temperature becomes lower.

Because states with lower energies correspond to desired atypical trajectories, we select a set of states whose energies $E$ are lower than a threshold $E_{cr} = -5$. We show these states in figure 4(a). By using cluster analysis, we divide these initial states into clusters. Because these clusters are well separated in the plane, we identify each cluster as a representation of a qualitatively different set of trajectories.

In each cluster, we identify an initial state that has minimum energy. Figure 4(b) shows atypical trajectories starting from these initial conditions on the $(\dot{\theta}_1, \dot{\theta}_2)$ plane. It is observed that each cluster corresponds to a qualitatively different pattern of motion. Examples of sequences of snapshots for patterns of the double pendulum are shown in figure 4(c), each of which corresponds to a trajectory obtained using the above procedure.

4. Parameter search and combined search

In this section, we discuss searching in a parameter space and combined searching in parameter and initial condition spaces as an extension of our method. Examples are sampling of the boundary of the Mandelbrot set and exploration of the global bifurcation structure of the logistic map.

4.1. Boundary of the Mandelbrot set

For a map $f_c(z) = z^2 + c$ parameterized by a parameter $c \in \mathbb{C}$, consider the sequence $(0, f_c(0), f_c(f_c(0)), \ldots)$. The Mandelbrot set [32] is defined as the set of points $c \in \mathbb{C}$ such that the above sequence does not escape to infinity. Hereafter, we use the notation $f_c(f_c(0)) = f_c^2(0)$ and $f_c(f_c(f_c(0))) = f_c^3(0)$, and so on.

The Mandelbrot set has an elaborate boundary in the complex plane, which does not simplify at any magnification. In order to compute the boundary of the set, we use the
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Figure 4. (a) States with $E < -5$ plotted on the $(\omega_1, \omega_2)$ plane. The states form clusters, which are regarded as sets of qualitatively different trajectories. Thirteen different clusters are identified by using cluster analysis, and they are plotted using different symbols indicated with numbers. (b) Typical trajectories starting from the state that has minimum energy within a cluster are plotted on the $(\dot{\theta}_1, \dot{\theta}_2)$ plane. Six trajectories are shown. The number indicates the cluster number in (a). (c) Sequences of snapshots of patterns of the double pendulum. Three trajectories, each of which converges to a different fixed point, are shown in the upper, middle, and lower panels. Each number in the panels indicates the cluster number in (a). The other parameters are the same as those in figure 3.

Parameter $c$ as a state of the proposed method and employ the following energy function:

$$E(c) = -\log(n(c)),$$

where the function $n(c)$ is defined as the smallest $n$ such that $|f^n_c(0)| > 2$. If $n > N$ for a prescribed large number $N = 200$, we set $n(c) = 1$ and $E(c) = 0$. In that case, the point $c$ is considered to be within the Mandelbrot set and not on the boundary.

Using this energy function, we calculated the boundary of the Mandelbrot set using our proposed method, the results of which are shown in figure 5. While the points are distributed almost randomly in the complex plane for replicas with a high temperature $1/\beta$, the distribution of points corresponding to replicas with lower temperatures is concentrated on the boundary of the Mandelbrot set.

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Figure 5. (a) The Mandelbrot set. The black region shows the Mandelbrot set and the outside of the set is colored according to the escape time. (b) The boundary of the Mandelbrot set. Six replicas with $\beta = 1.0, 2.0, 3.0, 4.0, 5.0,$ and $6.0$ are used for sampling. $N_{\text{min}} = 1$ and $N_{\text{max}} = 9$.

4.2. Periodic orbits and the bifurcation diagram of the logistic map

The logistic map [33,1] is defined by

$$f_a(x) = ax(1-x),$$

where $a \in [0, 4]$ is a parameter. Let us consider the energy function

$$E(a, x_0) = \log(|f_a^k(x_0) - x_0| + \epsilon),$$

where $k$ is a given period and $\epsilon$ is a constant that determines the minimum energy. Indeed, we can find initial conditions $x_0$ corresponding to period $k$ orbits for a given parameter $a$ using the energy function (9) using our proposed method (results not shown here). On the other hand, the extension of the sampling state space from $x_0$ to $(a, x_0)$ enables us to study the global bifurcation structure of periodic solutions. The extension is straightforward, i.e., we sample the vector $(a, x_0)$ from the Gibbs distribution determined by the same energy function (9) using REM.

In figure 6, the result for the period $k = 3$ is shown, where sampled points are plotted on the $(a, x_0)$ plane. We sample orbits from $a \in [3.8, 4]$ and $x \in [0, 1]$. The points are scattered broadly in the vicinity of the true bifurcation branch of the period $k = 3$ orbits at higher temperatures. The dispersion of the points becomes smaller at lower temperatures and the bifurcation structure of period three orbit is revealed.
Figure 6. The bifurcation structure of the period 3 solutions of the logistic map is obtained using our proposed method. Ten replicas are used with $\beta = 0.5i$ for $i = 1, 2, \ldots, 10$. $\epsilon = 10^{-4}$, $N_{\min} = 1$, and $N_{\max} = 11$. (a) $\beta = 0.5$. (b) $\beta = 1.0$.

5. Summary and discussion

In this paper, we have presented a general strategy for exploring unstable structures generated by non-linear dynamical systems. An artificial ‘energy’ is defined as a function of the initial condition of the trajectory, and the Gibbs distribution induced by the energy is sampled by the Metropolis method. When a suitable ‘energy’ is selected, sampling from the Gibbs distribution at low temperatures provides efficient sampling of rare initial conditions that leads to interesting trajectories. The replica exchange Monte Carlo (REM) is used to avoid capture in local minima of the energy landscape.

The implementation of our proposed method is simpler than those of methods in which the artificial energy is defined in the space of entire trajectories. With this advantage, our method can treat a variety of problems, including searching for unstable periodic orbits of the Lorenz model and for stable manifolds of unstable fixed points of a double pendulum.

We have also shown that searching in the parameter space and combined searching for initial conditions and parameters become possible upon adding the parameters to the state vector. Two examples shown here are the Mandelbrot set of a complex dynamical system and the bifurcation diagram of the logistic map.

An important future problem is that of calculating quantitative results using our proposed method. Examples include the relative densities of initial conditions that lead to different Lyapunov numbers and densities of the time of escape from a chaotic saddle. These calculations are possible because REM is not only an optimization method, but also provides correct sampling from the Gibbs distribution. It is also interesting to introduce other kinds of extended ensemble Monte Carlo methods such as multicanonical algorithms for this purpose. We are currently undertaking research in this area, and the results will be published elsewhere.

The combined search for initial conditions and parameters using our method is also promising and should be tested for the study of more complicated systems. There is, however, an inherent interpretation problem, i.e., the joint density in the direct
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product of the parameter space and initial condition space appears to not have a definite interpretation. Our proposed method is already useful for providing a rough sketch of the bifurcation diagram, but it will be better if we can give a physical meaning to the joint density.

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References

[1] Ott E, 2002 Chaos in Dynamical Systems (Cambridge: Cambridge University Press)
[2] Cvitanović P, Artuso R, Mainieri R, Tanner G, Vattay G, Whelan N and Wirzba A, Chaos—classical and quantum, http://chaosbook.org/ unpublished (web book)
[3] Landau D and Binder K, 2005 A Guide to Monte Carlo Simulations in Statistical Physics (Cambridge: Cambridge University Press)
[4] Newman M E J and Barkema G T, 1999 Monte Carlo Methods in Statistical Physics (Oxford: Oxford University Press)
[5] Liu J, 2001 Monte Carlo Strategies in Scientific Computing (Berlin: Springer)
[6] Young A P (ed), 1997 Spin Glasses and Random Fields (Singapore: World Scientific)
[7] Janke W (ed), 2008 Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules (Springer Lect. Notes Phys. vol 736) (Berlin: Springer)
[8] Mitsutake A, Sugita Y and Okamoto Y, Generalized-ensemble algorithms for molecular simulations of biopolymers, 2001 Biopolymers (Peptide Science) 60 96
[9] Cho A E, Doll J D and Freeman D L, The construction of double-ended classical trajectories, 1994 Chem. Phys. Lett. 229 218
[10] Bolhuis P G, Dellago C and Chandler D, Sampling ensembles of deterministic transition pathways, 1998 Faraday Discuss. 110 421
[11] Vlugt T J H and Smit B, On the efficient sampling of pathways in the transition path ensemble, 2000 Phys. Chem. Commun. 2 2
[12] Kawasaki M and Sasa S I, Statistics of unstable periodic orbits of a chaotic dynamical system with a large number of degrees of freedom, 2005 Phys. Rev. E 72 037202
[13] Sasa S I and Hayashi K, Computation of the Kolmogorov–Sinai entropy using statistical mechanics: application of an exchange Monte Carlo method, 2006 Europhys. Lett. 76 156
[14] Giardinà C, Kurchan J and Peliti L, Direct evaluation of large-deviation functions, 2006 Phys. Rev. Lett. 96 120603
[15] Tailleur J and Kurchan J, Probing rare physical trajectories with Lyapunov weighted dynamics, 2007 Nat. Phys. 3 203
[16] Bolhuis P G, Chandler D, Dellago C and Geissler P, Transition path sampling: throwing ropes over mountain passes, in the dark, 2002 Annu. Rev. Phys. Chem. 59 291
[17] van Erp T S, Reaction rate calculation by parallel path swapping, 2007 Phys. Rev. Lett. 98 268301
[18] Doucet A, De Freitas N and Gordon N (ed), 2001 Sequential Monte Carlo Methods in Practice (Berlin: Springer)
[19] Iba Y, Population Monte Carlo algorithms, 2001 Trans. Japan. Soc. Artif. Intell. 16 279
[20] Kaloš M H, Monte Carlo calculations of the ground state of three- and four-body nuclei, 1962 Phys. Rev. 128 1791
[21] Sweet D, Nusse H E and Yorke J A, Stagger-and-step method: detecting and computing chaotic saddles in higher dimensions, 2001 Phys. Rev. Lett. 86 2261
[22] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E, Equations of state calculations by fast computing machines, 1953 J. Chem. Phys. 21 1087
[23] Hukushima K and Nemoto K, Exchange Monte Carlo method and application to spin glass simulations, 1996 J. Phys. Soc. Japan 65 1604
[24] Iba Y, Extended ensemble Monte Carlo, 2001 Int. J. Mod. Phys. C 12 623
[25] Biham O and Wenzel W, Characterization of unstable periodic orbits in chaotic attractors and repellers, 1989 Phys. Rev. Lett. 63 819

doi:10.1088/1742-5468/2009/02/P02043
Exploration of order in chaos using the replica exchange Monte Carlo method

[26] Diakonos F K, Schmelcher P and Biham O, *Systematic computation of the least unstable periodic orbits in chaotic attractors*, 1998 Phys. Rev. Lett. 81 4349

[27] Davidchack R L and Lai Y-C, *Efficient algorithm for detecting unstable periodic orbits in chaotic systems*, 1999 Phys. Rev. E 60 6172

[28] Lan Y and Cvitanović P, *Variational method for finding periodic orbits in a general flow*, 2004 Phys. Rev. E 69 016217

[29] Lorenz E N, *Deterministic non-periodic flow*, 1963 J. Atmos. Sci. 20 130

[30] Sparrow C, 1982 *The Lorenz Equations: Bifurcations, Chaos, and Strange Attractors* (New York: Springer)

[31] Doedel E J, Paffenroth R C, Champneys A R, Fairgrieve T F, Kuznetsov Yu A, Sandstede B and Wang X, *AUTO 2000: continuation and bifurcation software for ordinary differential equations (with homcont)*, 2001 Technical Report, Caltech

[32] Mandelbrot B B, 2004 *Fractals and Chaos: The Mandelbrot Set and Beyond* (Berlin: Springer)

[33] May R, *Biological populations with nonoverlapping generations: stable points, stable cycles, and chaos*, 1974 Science 186 645

doi:10.1088/1742-5468/2009/02/P02043