Chaotic billiard dynamics for herding

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Abstract: Herding systems are discrete-time nonlinear dynamical systems designed efficiently for statistical inference. In this paper, we introduce a continuous-time version of these systems, which we call herding billiard systems. In contrast to the weakly chaotic dynamics of the original version, the continuous-time version is shown to have chaotic pseudo-billiard dynamics, while inheriting the fundamental sampling functions. We also present the connection between these two versions. Thus, herding billiard systems provide a novel approach to the complexity of herding systems from the viewpoint of chaotic billiard dynamics.

Key Words: herding system, pseudo billiard, piecewise isometry, chaos, statistical inference

1. Introduction

In the herding systems recently proposed by Welling [1, 2], statistical learning and inference are combined into one algorithm. The sequence of samples generated from the herding systems is assured to satisfy predefined statistics, and can be used to estimate other statistics of interest. The herding algorithm is very efficient compared with the conventional two-step approach that attempts to determine the parameters of a probabilistic model and obtain samples from the model.

A remarkable aspect of herding systems, especially from the viewpoint of nonlinear dynamics, is that the herding algorithm is completely deterministic; it is described as a discrete-time nonlinear dynamical system. More specifically, the dynamics of herding systems belongs to the class of piecewise isometries. As is the case for many piecewise isometries [3–10], the herding systems typically have complex dynamics with fractal attracting sets [1, 2]. However, the Lyapunov exponents of the dynamics are strictly zero, which does not seem to properly characterize the complexity of the dynamics. This is because the complexity originates solely from the discontinuities of the piecewise isometries.

In this paper, we introduce a continuous-time version of herding systems, which we call herding billiard systems, as they have pseudo-billiard dynamics. We show that the continuous-time systems naturally derived from the herding systems show chaotic behavior characterized by positive Lyapunov exponents. Although the dynamics is different, the continuous-time systems inherit fundamental sampling functions of the original herding systems. We also present the connection between these two versions. Thus, we present a novel approach to the complexity of herding systems from the viewpoint of chaotic billiard dynamics.

It should be noted that the billiard dynamics proposed in this paper is closely related to switched arrival systems [5,11–14], which were proposed as a simple model of production dynamics. The dynamics of switched arrival systems is described by chaotic pseudo-billiards, and the discretized
version is described by piecewise isometries with nontrivial complex dynamics [5]. This relation is analogous to that between the proposed billiard systems and herding systems. In fact, we show that the switched arrival systems can be regarded as a variant of the herding billiard systems. Thus, our study extends the relation between pseudo-billiard dynamics and piecewise isometries.

2. Herding system

The problem we consider here is to obtain a sequence of samples \( s^{(1)}, s^{(2)}, \ldots \) from a finite set of symbols \( S \). For each symbol \( s \in S \), the corresponding feature vector \( \phi(s) = (\phi_1(s), \ldots, \phi_N(s))^T \in \mathbb{R}^N \) is given. The sequence is required to satisfy the constraint such that the feature vector \( \phi(s^{(t)}) \) averaged over the sequence coincides with the predefined target vector \( \mu \). If a sequence of plausible samples is obtained, it can be used to estimate other statistics of interest.

To obtain a sequence, we normally find appropriate parameter values of a probabilistic model, and draw samples from that model. As parameters, let us define the weight vector \( w = (w_1, \ldots, w_N)^T \) associated with the feature vectors. The weight vector is determined such that the Gibbs distribution with respect to the energy function \( E(s, w) = -w^T \phi(s) \) achieves the maximum entropy under the predefined constraint. Unfortunately, this learning process requires lengthy computation. Moreover, even if the optimal weight vector is obtained, the Markov-chain Monte Carlo (MCMC) process for generating samples may get stuck due to the multimodal distribution of the model.

In herding systems [1, 2], learning of the model and sampling from the model are integrated; the system keeps updating the weight vector \( w^{(1)}, w^{(2)}, \ldots \) while generating samples \( s^{(1)}, s^{(2)}, \ldots \). Specifically, the herding system generates a sample \( s^{(t+1)} \) and updates the weight vector \( w^{(t+1)} \) at time \( t + 1 \) as follows:

\[
\begin{align*}
\text{(1)} \quad s^{(t+1)} &= \arg\max_{s \in S} w^{(t)^T} \phi(s), \\
\text{(2)} \quad w^{(t+1)} &= w^{(t)} + \mu - \phi(s^{(t+1)}).
\end{align*}
\]

Note that this process can be understood as a gradient ascent algorithm for \( w \) with respect to the function

\[
G(w) = w^T \mu - \max_s w^T \phi(s),
\]

which is called a Tipi function [1]. As shown in Fig. 1, function \( G(w) \) is continuous, piecewise linear, non-positive, concave, and scale free in the sense that \( G(\alpha w) = \alpha G(w) \) for any \( \alpha \geq 0 \). It has a maximum at the origin, \( G(0) = 0 \), and the weight vector \( w^{(t)} \) keeps moving around the origin without converging. An example of the attracting set of the weight vector is shown in Fig. 2.

![Fig. 1. Tipi function \( G(w) \) of a two-dimensional herding system. The feature vectors and the target vector are described in Section 4.1. The two-dimensional state space is divided into five regions by the symbols that minimize the energy function. The red polygon shows the contour line at \( G(w) = -1 \).](image)
Fig. 2. Dynamics of a two-dimensional herding system. The system is the same as Fig. 1. The attracting set shown by the red points has a fractal structure. Five regions, each corresponding to one of the five symbols, are indicated by the dashed lines.

The difference between the predefined target vector $\mu$ and the feature vector averaged over samples generated until time $T$ is given by

$$
\mu - \frac{1}{T} \sum_{t=1}^{T} \phi(s(t)) = \frac{1}{T}(w(T) - w(0)).
$$

The right-hand side goes to zero as $T \to \infty$, because it can be shown that the sequence $w(t)$ wanders within a bounded set. Therefore, the herding system is assured to generate a sequence of samples satisfying the predefined features asymptotically. Moreover, it has the prominent convergence rate in the order of $1/T$, which is much faster than $1/\sqrt{T}$ of random sampling algorithms such as MCMC.

From the viewpoint of nonlinear dynamics, herding systems belong to the class of piecewise isometries; the state space can be divided into regions by the symbol $s$ that minimizes the energy function, and in each region, its dynamics is merely a translation by a constant vector $\mu - \phi(s)$. It is known that piecewise isometries generally have complex dynamics and fractal attracting sets despite the Lyapunov exponents strictly equal to zero [3–10]. Herding systems also have fractal attracting sets, as shown in Fig. 2. Owing to the complex dynamics of herding systems, sequences of samples generated from these systems generally have a certain amount of randomness, and the empirical distribution of samples have relatively high entropy.

Herding systems in a one-dimensional weight space (i.e., $N = 1$) have dynamics of a rigid rotation, and yield a Sturmian sequence when the rotation is irrational. From the viewpoint of signal processing, one-dimensional herding systems can be regarded as a $\Delta\Sigma$-modulator [15] or an error diffusion algorithm [16] with a constant input. Note that the herding algorithm works without any problem even if the target feature vector $\mu$ in Eq. (2) is time-dependent [17]. Therefore, herding systems can be considered as a natural extension of these signal processing systems.

3. Herding billiard system

Now we consider a continuous-time version of herding systems. The system presents a symbol continuously and changes it to another irregularly; let $t_1$, $t_2$, ... be the sequence of the switching times. Let $s_k$ denote the symbol presented from time $t_k$ to $t_{k+1}$, and $\tau_k$ denote the time interval $t_{k+1} - t_k$. Then the feature vector averaged from time $t_1 = 0$ to $t_{K+1} = T$ is represented by

$$
\hat{\mu} = \frac{1}{T} \int_{0}^{T} \phi(s(t))dt = \frac{1}{T} \sum_{k=1}^{K} \tau_k \phi(s_k).
$$
In a sense, the system is considered to produce a discrete-time sequence of samples $s_1, s_2, \ldots$ weighted by the time intervals $\tau_1, \tau_2, \ldots$. In any case, the problem is to generate such a sequence of symbols that satisfies $\hat{\mu} = \mu$.

The dynamics of the weight vector $w$ in the continuous-time version is given by the following differential equation:

$$\frac{dw}{dt} = \mu - \phi(s), \quad (6)$$

which is natural from Eq. (2). To confine the weight vector in a bounded region, we define a billiard table as $P = \{w : G(w) \geq -1\}$ using the Tipi function $G(w)$ (see Eq. (3) and Fig. 1). Note that $-1$ can be arbitrary negative value. The symbol $s$ changes when and only when $w$ reaches the boundary of the billiard table $\partial P = \{w : G(w) = -1\}$ as follows:

$$s := \arg\max_{s' \in S} w^T \phi(s') \quad \text{when} \quad w \in \partial P. \quad (7)$$

Then, the weight vector $w$ reflects to the inside of the billiard table $P$, because according to Eq. (6), it reflects exactly to the gradient direction of the function $G(w)$.

As in the case of the discrete-time herding system, the difference between the predefined target vector $\mu$ and the feature vector averaged over samples generated until time $T$ is given by

$$\mu - \hat{\mu} = \frac{1}{T} \int_0^T (\mu - \phi(s)) dt = \frac{1}{T} (w(T) - w(0)), \quad (8)$$

which means that $\hat{\mu}$ converges to $\mu$ as $T \to \infty$ with the rate in the order of $1/T$, because $w(t)$ is always within the bounded billiard table $P$.

In the billiard table $P$, the weight vector $w$ moves at a constant velocity according to Eq. (6), and changes its direction according to Eq. (7) at the boundary $\partial P$ of the table. Therefore, the dynamics can be understood as a pseudo billiard [14]. Figure 3 shows the billiard table and a trajectory of the herding billiard system corresponding to the herding system shown in Fig. 2.

The billiard dynamics induces a Poincaré map $w(t_k) \mapsto w(t_{k+1})$ on the boundary of the table. The map is piecewise linear. Moreover, it can be shown that perturbations to the states essentially grow in time. See Appendix for the details of the Poincaré map.

![Fig. 3. Dynamics of a two-dimensional herding billiard system. The feature vectors and the target vector are the same as Figs. 1 and 2. The black solid line shows the boundary of the billiard table, which is defined as the contour line at $G(w) = -1$ (the red polygon in Fig. 1). The red lines inside the billiard table show a trajectory for 100 iterations of the Poincaré map.](image-url)
4. Numerical experiments

4.1 Two-dimensional herding system

Let us consider the case that feature vectors are two-dimensional ($N = 2$). In this case, the herding dynamics of the weight vectors is in a polygon on the two-dimensional plane, and the billiard dynamics is reduced to a one-dimensional Poincaré map.

In the example shown in Figs. 1, 2, and 3, we consider a system for five symbols $S = \{1, 2, 3, 4, 5\}$. The feature vectors for $s \in S$ are defined as $\phi(s) = (\cos 2\pi s/5, \sin 2\pi s/5)^	op$. We set the target feature vector as $\mu = (0.2, 0.2)^	op$.

The Poincaré map of the billiard system represented as an interval map is shown in Fig. 4(a); the boundary of the table $P$ shown in Fig. 3 is cut at the upper-right vertex and opened up, and the coordinate $x(k)$ is defined as the distance from the upper-right corner to $w(t_k)$ measured along the boundary counterclockwise. As shown in Fig. 4(a), the Poincaré map from $x(k)$ to $x(k + 1)$ is piecewise linear and expanding; the gradients are all negative and less than $-1$. Hence, the map has no stable periodic points, and the Lyapunov exponent of any orbit is positive. The Lyapunov exponent of the Poincaré map is numerically estimated as 0.1683. The empirical distribution of the orbits of the Poincaré map is shown in Fig. 4(b). These numerical results indicate that the system is chaotic.

The distribution of samples obtained from the systems are shown in Table I. The original herding system achieves a high entropy value very close to the optimum. The entropy for the billiard system is lower, but not very far from the optimum. Thus, the billiard system approximately inherits the sampling behavior of the original herding system, and yields samples with relatively high entropy.

4.2 Full-dimensional herding system

Let us consider another example in which probabilities for all the symbols are given. We assume that
Table I. Distribution of samples obtained from the herding billiard system (billiard) and the original herding system (herding), compared with the distribution with the maximum entropy (optimum). The distribution is calculated from $10^6$ iterations of the systems.

|        | 1     | 2     | 3     | 4     | 5     | entropy [bits] |
|--------|-------|-------|-------|-------|-------|---------------|
| billiard | 0.260 | 0.206 | 0.091 | 0.121 | 0.322 | 2.184         |
| herding | 0.313 | 0.171 | 0.094 | 0.151 | 0.271 | 2.203         |
| optimum | 0.311 | 0.167 | 0.102 | 0.141 | 0.279 | 2.204         |

Figure 5. Average absolute errors of the herding billiard system (billiard; red lines), the original herding system (herding; blue lines), and random sampling (random; black dashed lines). The initial state $w(0)$ of the billiard system is drawn from the uniform distribution on $[-1, 1]^N$. (a) First 1000 iterations. (b) The log-log plot for $10^5$ iterations.

Symbols in $S = \{1, \ldots, N\}$ appear with probabilities $p_1, \ldots, p_N$. The feature vector $\phi(s)$ is defined as the $s$th standard basis vector for $N$-dimensional Euclidean space, and the target vector is set as $\mu = (p_1, \ldots, p_N)$. Then, the herding system is written as follows:

$$s^{(t+1)} = \arg\max_{s \in S} w_s^{(t)},$$  \hspace{1cm} (9)

$$w_i^{(t+1)} = w_i^{(t)} + p_i - \delta_i(s^{(t+1)}) \quad (i = 1, \ldots, N),$$  \hspace{1cm} (10)

where $\delta$ is Kronecker’s delta function. The corresponding herding billiard system is as follows:

$$\frac{dw_i}{dt} = p_i - \delta_i(s(t)) \quad (i = 1, \ldots, N),$$  \hspace{1cm} (11)

$$s(t) := i \quad \text{when} \quad -w_i + \sum_s w_s p_s = -1.$$  \hspace{1cm} (12)

Figure 5 shows the results of numerical experiments for $N = 100$. The experiments are performed for a target feature vector chosen in the same way as in Fig. 3 of Ref. [2]; that is, the target vector $\mu$ is determined by drawing 100 values from the uniform distribution on $[0, 1]$ and normalizing them. In Fig. 5, the average absolute errors for the herding billiard system (Eqs. (11) and (12)), the original herding system (Eqs. (9) and (10)), and random i.i.d. sampling are shown. Figure 5(a) shows that,
initially, the performance of the herding billiard system is similar to that of random sampling. However, Fig. 5(b) shows that its asymptotic performance indicated by the gradient of the log-log plot is the same as the original herding system. Thus, the herding billiard system inherits the asymptotic behavior of the original herding system in the sense that the error decreases in the order of $1/T$, which is faster than the order $1/\sqrt{T}$ of random sampling.

This full-dimensional herding system is closely related to switched arrival systems \[11\]. If we define a modified billiard table as $P_{E} = \{w : \min_{s} E(s, w) \geq -1\}$, the state switches when $w_{i}(t) = 1$. Then the billiard dynamics is exactly the same as that of the switched arrival system with $N$ tanks, if we regard $1 - w_{i}(t)$ as the water level of the $i$th tank.

5. Discussion

Dynamics of the herding billiard systems is different from the original herding systems; the billiard systems have continuous-time chaotic dynamics, while the original systems have discrete-time non-chaotic (or weakly chaotic) dynamics. However, these two types of systems can be seamlessly related to one another, by considering re-discretization of the billiard systems.

Re-discretization of a herding billiard system (Eqs. (6) and (7)) with the discretization time step $\Delta t$ yields the following piecewise isometry:

\[
s^{(t+1)} = \begin{cases} 
  s^{(t)} & \text{if } w^{(t)} \in P, \\
  \arg \max_{s \in S} w^{(t)}^{\top} \phi(s) & \text{if } w^{(t)} \notin P,
\end{cases}
\]

\[
w^{(t+1)} = w^{(t)} + (\mu - \phi(s^{(t+1)})) \Delta t.
\]

Note that in the discretized system, the weight vector $w$ jumps over the boundary. Switching of the symbols occurs only when state $w$ goes out of the table, similarly to the discretization of switched arrival systems in Ref. [5]. Even in the one-dimensional case, the dynamics of the discretized billiard system reduces to double rotations [7] that have nontrivial complex dynamics [8].

The obtained discrete-time dynamics depends on the time step $\Delta t$, and is different from the original herding system. However, if we change the scale of $w$ and replace $w/\Delta t$ by $w$, these equations can be rewritten as follows:

\[
s^{(t+1)} = \begin{cases} 
  s^{(t)} & \text{if } w^{(t)} \in P/\Delta t, \\
  \arg \max_{s \in S} w^{(t)}^{\top} \phi(s) & \text{if } w^{(t)} \notin P/\Delta t,
\end{cases}
\]

\[
w^{(t+1)} = w^{(t)} + \mu - \phi(s^{(t+1)}).
\]

Here, note that Eq. (16) coincides with Eq. (2) of the original herding system.

In the limit of $\Delta t \to 0$, the dynamics described by Eqs. (13) and (14) goes to the continuous-time dynamics of the herding billiard system. On the other hand, in the limit of $\Delta t \to \infty$, the dynamics described by Eqs. (15) and (16) goes to the original herding system, because the billiard table $P/\Delta t$ shrinks to the origin and $w$ never visits inside the table $P/\Delta t$ of Eq. (15). Therefore, the dynamics of the herding billiard systems and the original herding systems coincide with the two limiting regimes of $\Delta t \to 0$ and $\Delta t \to \infty$, respectively, and seamlessly related to one another by changing the time step $\Delta t$ of the re-discretized system.

For intermediate values of time step $\Delta t$, the discretized dynamics described by Eqs. (15) and (16) can be understood as a moderate variant of herding systems; the minimization step for finding a new sample (Eq. (1)) is performed only when $w$ is sufficiently far away from the origin. In this sense, the two systems can also be seamlessly related to one another by changing the moderateness for finding new samples.

The continuous-time dynamics of herding billiard systems is determined solely by the shape of the billiard table $P$, because the billiard ball hitting the boundary of the table bounces to the direction normal to the boundary. Therefore, the relation between the shape and the pseudo-billiard dynamics would be interesting, as has been studied for normal elastic billiard dynamics.
There are several other types of sampling algorithms based on chaotic dynamics. Recently, it was shown that chaotic pseudo-billiard dynamics [18–20] can simulate probabilistic spin systems such as the Ising model and Boltzmann machines. As another example, there is an intriguing series of studies on chaotic Monte Carlo algorithms, which achieve superefficient convergence rates faster than $1/T$ (see, e.g., Ref. [21]). These chaotic sampling algorithms are expected to be good examples for reconsidering the roles of random numbers and deterministic chaos in statistical methods.

6. Summary
To summarize, we introduced a continuous-time version of herding systems. The continuous-time version inherits the fundamental sampling functions of the original herding systems; it yields samples with relatively high entropy, and the error decreases in the order of $1/T$. Considering the connection between the dynamics of two versions, herding billiard systems provide a novel approach to the complexity of herding systems from the viewpoint of chaotic billiard dynamics.

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Appendix
A. Poincaré map
In this appendix, we derive the Poincaré map of the herding billiard system induced on the boundary of the billiard table. Assume that the weight vector $w(t_k) \in P$ and the symbol $s_k \in S$ at time $t_k$ are given. Then since $w(t_{k+1}) \in \partial P$ at time $t_{k+1}$, we have

$$v(s_{k+1})^T w(t_{k+1}) = -1,$$

$$w(t_{k+1}) = w(t_k) + v(s_k) \tau_k,$$

where $v(s) = \mu - \phi(s)$. Then, $\tau_k$ is obtained as

$$\tau_k = -\frac{v(s_{k+1})^T w(t_k) + 1}{v(s_{k+1})^T v(s_k)}.$$

Therefore, the Poincaré map is given as follows:

$$w(t_{k+1}) = w(t_k) - \frac{v(s_k)}{v(s_{k+1})^T v(s_k)} v(s_{k+1})^T w(t_k) + 1$$

$$= \left( I - v(s_k) v(s_{k+1})^T v(s_k) \right) w(t_k) - \frac{v(s_k)}{v(s_{k+1})^T v(s_k)} v(s_{k+1})^T v(s_k).$$

In the iteration of this linear map, the effect of a perturbation $\Delta w(t_k)$ to the state $w(t_k) \in \partial P$ essentially grows in time as follows:

$$|\Delta w(t_{k+1})|^2 = \left| \left( I - \frac{v(s_k) v(s_{k+1})^T v(s_k)}{v(s_{k+1})^T v(s_k)} \right) \Delta w(t_k) \right|^2$$

$$= \Delta w(t_k)^T \left( I - \frac{v(s_k) v(s_{k+1})^T v(s_k)}{v(s_{k+1})^T v(s_k)} \right) \left( I - \frac{v(s_k) v(s_{k+1})^T v(s_k)}{v(s_{k+1})^T v(s_k)} \right) \Delta w(t_k)$$

$$= |\Delta w(t_k)|^2 + \frac{v(s_k) v(s_{k+1})^T v(s_k)}{v(s_{k+1})^T v(s_k)} |\Delta w(t_k)|^2 \geq |\Delta w(t_k)|^2,$$

because $v(s_k)^T \Delta w(t_k) = 0$. This means that all the Lyapunov exponents in the Lyapunov spectrum are non-negative. Furthermore, there exists $\Delta w(t_k)$ such that $|\Delta w(t_{k+1})| > |\Delta w(t_k)|$ unless $v(s_k) \propto v(s_{k+1})$. Therefore, we can generally expect that the largest Lyapunov exponent is positive.
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