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Investigation of the statistical distance to reach stationary distributions

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ABSTRACT

The thermodynamic length gives a Riemannian metric to a system's phase space. Here we extend the traditional thermodynamic length to the information length ($\mathcal{L}$) out of equilibrium and examine its properties. We utilise $\mathcal{L}$ as a useful methodology of analysing non-equilibrium systems without evoking conventional assumptions such as Gaussian statistics, detailed balance, priori-known constraints, or ergodicity and numerically examine how $\mathcal{L}$ evolves in time for the logistic map in the chaotic regime depending on initial conditions. To this end, we propose a discrete version of $\mathcal{L}$ which is mathematically well defined by taking a set theoretic approach. We identify the areas of phase space where the loss of information of the system takes place most rapidly. In particular, we present an interesting result that the unstable fixed points turn out to most efficiently drive the logistic map towards a stationary distribution through $\mathcal{L}$.

1. Introduction

A major goal in statistical mechanics is to understand how non-equilibrium systems evolve in time. The main reason this is a difficult problem is that much of the theory and machinery of traditional Boltzmann Gibbs statistics does not carry over to the non-equilibrium regime. Furthermore, non-equilibrium systems are not guaranteed to have well-defined time-independent constraints which can be utilised in the determination of the form of the probability density functions (PDFs). Another important issue which is addressed in this manuscript is the amount of phase space in the course of a system's (e.g. rapid) time-evolution, as they are not guaranteed to have explored all possible states in the phase space, invalidating any assumption of ergodicity. Thus, the presence (or, existence) of phase space with zero probabilities is a potential problem for any system starting from a set of non-equilibrium conditions.

A general measure that has proven to be very appealing theoretically is the thermodynamic length ($\mathcal{L}_{th}$). The thermodynamic length endows a phase space with a Riemannian metric, thus allowing one to measure the "distance" that a system travels between thermodynamic equilibrium states. These systems are governed by a set of control parameters λ^i which are the experimentally controllable variables of the system, the thermodynamic length is defined as,

$$\mathcal{L}_{th} = \int_0^\tau dt \sqrt{\frac{d\lambda^i}{dt} g_{ij} \frac{d\lambda^j}{dt}}. \tag{1}$$

The metric g_{ij} depends on the parameters of the system being analysed. Most previous studies used thermodynamic functions to define g_{ij} based on equilibrium states. For instance, Weinhold [19] used $g_{ij} = d^2U(V,S,N)/dx_i dx_j$ ($x_i = U, V, N$ for $i = 1, 2, 3$), where U is the internal energy which is a function of the extensive variables. In comparison, Rupeiner [14] used the second derivative of the entropy with respect to extensive variables (for other examples see [2,5,12]). Out of equilibrium the control parameters are often not known, making Weinhold and Rupeiner's metrics inapplicable. Thus, we take the approach of Crook's [3] and use the probability distribution function $p(x,t)$ to define the Fisher information matrix [6] as follows:

$$g_{ij} = \sum_x p(x,t) \frac{\partial \log p(x,t)}{\partial \lambda^i} \frac{\partial \log p(x,t)}{\partial \lambda^j}. \tag{2}$$

Here $p(x,t)$ is the probability of finding the system in "state" x at time t, given that it evolved from an initial distribution $p(x,t_0)$ at an earlier time, $t > t_0$ and the conservation of total probability requires $p(x,t)$ follow, $\sum_x p(x,t) = 1$. The control parameters λ^i specify how the system evolves through the surface of accessible states specified by λ^i. In equilibrium thermodynamics these could be for example the temperature or pressure of the system [3].

As we will see in the next section, putting Eq. (2) into Eq. (1) and summing over λ^i and λ^j gives us a distance in terms of probability distributions. It is important to note that Eq. (2) in general

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fulfils the requirements of a metric either whether the system is in equilibrium or not. Interestingly, in thermal equilibrium, using g_{ij} of Eq. (2) in Eq. (1) gives that $\mathcal{L}$ is proportional to the covariance of the forces conjugate to control parameters λ^i. That is, in equilibrium, thermodynamic length can be thought of as an integral in time over the fluctuations the system undergoes (see, e.g. [3]). Out of equilibrium, this is no longer true, and Eq. (2) is instead related to the integral of the covariance of fluctuations at different times [18].

A large body of theoretical work has already been developed for the thermodynamic length, starting with Weinhold [19], Rupeiner [14] and Schlögl [16], continuing with [4] among others. There is however a distinct lack of numerical illustrations for the thermodynamic length. This is partly caused by the computational demand in time and difficulties associated with obtaining PDFs which are sufficiently accurate.

When our system evolves over a manifold of non-equilibrium states we will use the information length ($\mathcal{L}$) instead of the thermodynamic length. Using $\mathcal{L}$ the relaxation of an arbitrary configuration of the system will be numerically investigated as it relaxes to a stationary distribution. In this work stationary does not imply equilibrium, as equilibrium also requires the system satisfy detailed balance (as defined in Section 3). In particular, we use a discrete map (the logistic map) as a typical example of a non-equilibrium system which also allows us to take computational advantages, as the simulation of maps is much less demanding and time-consuming than continuous systems. As noted above, for any non-equilibrium system having zero-valued probabilities $\mathcal{L}$ can be undefined. To overcome this we propose a discrete version of $\mathcal{L}$ which is mathematically well defined by taking a set theoretic approach.

The paper is organised as follows. Section 2 introduces the information length and provides its key properties in detail along with the definitions of our sets. These are followed in Section 3 where we show that $\mathcal{L}$ must increase for any PDFs other than the invariant (stationary) distribution. Section 4 will numerically examine the information length for the logistic map in the chaotic regime. In particular, using the logistic map we identify the areas of phase space where the conversion of the information of the system into work takes place most rapidly. We also show that the logistic map very often follows the path of minimum length. That is, the system follows the path of minimum information change. The importance of the minimum/optimal path has been noted in previous studies. For instance, J. Nulton et al. utilised this concept to link the thermodynamic length between equilibrium states to the "optimal" path in annealing processes [11]. In [5] it was suggested that experiments using biological motors would yield paths of minimum length. Conclusions are provided in Section 5.

2. Information length

To follow the path of a general non-equilibrium ensemble (e.g. as it evolves towards equilibrium), we measure the Fisher–Rao information by using Eq. (2) in Eq. (1) and define the information length as follows,

$$\mathcal{L} = \int_0^\tau dt \sqrt{\sum_x \frac{1}{p(x,t)}\left[\frac{dp(x,t)}{dt}\right]^2}. \tag{3}$$

Now distances are measured by the difference between consecutive PDFs. The difference in PDFs gives a measure of the statistical distance [11,20]. The evolution of a system can then be envisioned as the trajectory in the probability space where the distance/metric at different times is provided by the statistical distance. As time is the only parameter, Eq. (3) is ideally suited for analysing experimental data, which we use exclusively in the remainder of the paper.

An alternative expression to Eq. (3) is often necessary to describe the evolution of non-equilibrium systems since $\mathcal{L}$ is undefined for PDFs with zero values (i.e. when $p(x,t)=0$), as it is written in Eq. (3). This problem can be readily remedied by expressing $\mathcal{L}$ in terms of $q=\sqrt{p}$, as suggested by Wootters [20], which transforms Eq. (3) into the following form,

$$\mathcal{L} = 2\int_0^\tau dt \sqrt{\sum_x \left(\frac{dq(x,t)}{dt}\right)^2}, \tag{4}$$

which no longer has this singularity problem. However if time is discrete, Eq. (4) is not equivalent to Eq. (3), making it necessary to look for a different form of $\mathcal{L}$. Thus, in this paper, we propose a set theoretical approach to overcome this problem, as presented shortly.

To this end, we utilise a discrete version of Eq. (3),

$$\mathcal{L} = \sum_{t=1}^{\tau} \Delta t \sqrt{\sum_x \frac{1}{p(x,t)}\left(\frac{\Delta p(x,t)}{\Delta t}\right)^2} = \sum_{t=1}^{\tau} \Delta\mathcal{L}(t)\Delta t. \tag{5}$$

Here, $\Delta p(x,t) = p(x,t') - p(x,t)$ where $t' = t+1$. Note that for discrete systems, t simply denotes the iteration number, taking the integer values as $t = 1, 2, \ldots, \tau$ where τ is the total time of a given evolution. Consequently, for most of this work the time step Δt is 1. That is, $p(x,t')$ ($t' = t+1$) and $p(x,t)$ are the two consecutive PDFs (i.e. the probability of being in state x at time t' or t, respectively) while $\Delta p(x,t) = p(x,t') - p(x,t)$ is the difference between these two consecutive PDFs. As we are dealing with numerical simulations, our state space $\mathbf{X}$ will be coarse grained into a finite number of disjoint sets x, which represent the new "states" of the system. For the logistic map, examined shortly, x is a one dimensional variable, $x \in [-1, 1]$. The probability of being in "state" x at time t is then, $p(x,t)$, where, $\sum_x p(x,t) = 1$. It is straightforward to generalise x to any higher dimensions, $\mathbf{x} = \{x_i, x_j, \ldots, x_N\}$.

To guarantee that $\mathcal{L}$ is well defined for arbitrary discrete non-equilibrium systems, we need to account for states that have zero probability of being occupied along the system's evolution. That is, given a total state space $\mathbf{X}$, the probability of finding the system $p(x,t)$ in a particular states x can be zero ($p(x,t)=0$ for some $x \in \mathbf{X}$). As a result we define the following two sets depending on the evolution of PDFs at two consecutive times t and t' as

$$\begin{aligned} Q_p &= \left\{x : p(x,t) \neq 0 \;\middle|\; p(x,t') = 0\right\}, \\ Q_w &= \left\{x : p(x,t) \neq 0 \;\middle|\; p(x,t') \neq 0\right\}. \end{aligned} \tag{6}$$

One possibility that is not included in the above equation is the case where $p(x,t)=0$ and $p(x,t') \neq 0$, which can however be shown to have no contribution to $\mathcal{L}$. The subscript p in Q_p designates the unused probability of evolving over one time step, while w is the set that gives a measure of the available work in evolving over one time step, as shown later. To isolate the separate contributions to $\mathcal{L}$ from Q_p and Q_w, we define

$$L_{Q_p} = \sum_{x \in Q_p} \frac{p(x,t)}{(\Delta t)^2},$$

$$L_{Q_w} = \sum_{x \in Q_w} \frac{1}{p(x,t)}\left(\frac{\Delta p(x,t)}{\Delta t}\right)^2,$$

and express Eq. (5) as:

$$\mathcal{L} = \sum_{t=1}^{\tau} \Delta t \sqrt{L_{Q_p} + L_{Q_w}}. \tag{7}$$