Action principle and Jaynes’ guess method

Q.A. Wang

Institut Supérieur des Matériaux et Mécaniques Avancés, 44, Avenue F.A. Bartholdi, 72000 Le Mans, France

Abstract

A path information is defined in connection with the probability distribution of paths of nonequilibrium hamiltonian systems moving in phase space from an initial cell to different final cells. On the basis of the assumption that these paths are physically characterized by their action, we show that the maximum path information leads to an exponential probability distribution of action which implies that the most probable paths are just the paths of stationary action. We also show that the averaged (over initial conditions) path information between an initial cell and all the possible final cells can be related to the entropy change defined with natural invariant measures for dynamical systems. Hence the principle of maximum path information suggests maximum entropy and entropy change which, in other words, is just an application of the action principle of classical mechanics to the cases of stochastic or instable dynamics.

1 Introduction

The principle of maximum information and entropy are investigated for nonequilibrium hamiltonian system in connection with action principle of classical mechanics.

The entropy defined by Clausius is an equilibrium quantity[1] which are related later by Boltzmann and Gibbs to equilibrium probability distributions with \( S = \ln v \) and \( S = - \sum_{i=1}^{v} p_i \ln p_i \), respectively, here \( p_i \) is the normalized (\( \sum_{i=1}^{v} p_i = 1 \)) probability for the system to be found at state \( i \), \( v \) is the total number of states in the phase space occupied by the system (let Boltzmann
constant be unity). The methodology of the statistical mechanics based on Boltzmann and Gibbs entropies is later complemented by the principle of maximum entropy\(^1, 2\) which stipulates that the “best” equilibrium probability distributions should maximize Clausius entropy. This method was already used by Boltzmann and Gibbs\(^1, 3\). But thanks to the efforts of Jaynes\(^{14}\), it has been nowadays widely recognized to be a powerful inference method for guessing (not deriving) correct probability distributions of equilibrium as well as nonequilibrium systems. It should be noticed that one of the underlying philosophical significations of this method is the anthropomorphic aspect of entropy and information. They are not objective physical quantities. They are related to the ignorance of the observers. They can be used only for guessing, but not deriving probability\(^{14}\).

On the other hand, compared to equilibrium systems, the statistical and informational methodology for dynamical (nonequilibrium) systems seems less certain. We have seen recently the extension of the Boltzmann and Gibbs entropies to nonequilibrium systems (in local equilibrium or not)\(^4, 5, 6\). But as for the inference or guessing methods of nonequilibrium distributions, although it was assumed by Jaynes that the maximum entropy method always applied, the principle of minimum entropy production\(^7\) has been proposed for the systems sufficiently close to equilibrium state. For certain systems far from equilibrium, e.g., in the context of the climate of earth, we have still the principle of maximum entropy production (or minimum entropy exchange)\(^8, 9\). Here the entropy is always in the sense of Clausius, so the entropy production \(dS_i \geq 0\) according to the second law. Over the last years, we have seen the development of a nonextensive statistics which suggests that the Havrda-Charvat-Daroczy-Tsallis entropy\(^{10}\) should be maximized for nonequilibrium systems\(^{11, 12, 13}\), a new extension of Jaynes method to dynamical systems.

So we have before us many different even opposite methods for dynamical systems. Why do we have to maximize or minimize entropy or its production for equilibrium as well as nonequilibrium systems in variational inference method? Are information and entropy merely anthropomorphic quantities which have nothing to do with physical laws? Indeed, Jaynes method is not theoretically proved in spite of its success in “guessing” probability distributions. It is only supported by plausible arguments such as, e.g., “if a system is in a state with lower entropy it would contain more information than previously specified”, or “higher entropy states are more probable” and “less predictable”, etc\(^{1, 14}\). So maximum entropy is only considered as a princi-
ple of guess, but not deduction method of mechanics. The central quantities of this method, i.e., entropy and information, are only anthropomorphic[14], not objective quantities involved in fundamental laws of physics.

In this work, Jaynes approach is revisited under a different angle in connection with the principle of least (stationary) action. It will be shown that, for stochastic or instable dynamics of hamiltonian systems, maximum information and entropy must be used to derive correct probability distributions just as the least (stationary) action principle must be used for regular dynamics to derive the correct motions. We finally reach the conclusion that the anthropomorphic aspect of entropy and information is not needed in order to be able to maximize them for inference and correct guess. Maximum entropy is in fact a deductive method for deriving probability distributions. It is an application of the fundamental action principle of classical mechanics to probabilistic dynamics.

2 Assumptions and definitions

Let us begin by some assumptions and definitions concerning dynamical systems.

1. We recall that a phase space $\Gamma$ of thermodynamic system is defined such that a physical state of the system is represented by a point in that space. A phase volume $\Omega$ can be partitioned into $v$ cells of volume $s_i$ with $i = 1, 2, ... v$ in such a way that $s_i \cap s_j = \emptyset (i \neq j)$ and $\bigcup_{i=1}^{v} s_i = \Omega$. A state of the system can be represented by a sufficiently small phase cell in coarse graining way. The movement of a dynamical system can be represented by its trajectories (in the sense of classical mechanics) in $\Gamma$ space.

2. The natural invariant measure[15] $\mu_i$ is defined as the probability distribution for a nonequilibrium system to visit different elementary cells $i$ of its partitioned phase space.

3. The information we address in this work is a measure of the uncertainty of dynamical process. According to Shannon, this information can be calculated by the formula

$$H = - \sum_{k=1}^{v} p_k \ln p_k$$

(1)
with respect to certain probability distribution $p_k$ of that process and the index $k$ is summed over all the possible situations.

4. The entropy $S$ of a nonequilibrium system is defined with the natural invariant measure $\mu_i$ by

$$S = -\sum_{i=1}^{\nu} \mu_i \ln \mu_i.$$  

(2)

If this system reaches equilibrium at the end of a nonequilibrium process and has $\mu_i$ as its final probability distribution, then $S$ can be considered as the entropy in the sense of second law (Clausius).

3 A path information

In a previous work[16], we defined a path information for dynamical systems moving, over a large period of time, in the $\Gamma$-space between two points, $a$ and $b$, which are in two elementary cells of a given partition of the phase space. This path information is given by the Shannon formula with respect to the probability $p_k(b|a)$ for the system to take the path $k$ from the cell $a$ to the cell $b$ during $t_{ab}(k)$, as shown in Figure 1(I).

By definition, $p_k(b|a)$ is a transition probability from state $a$ to state $b$ via path $k$. We have $\sum_{k=1}^{\nu} p_k(b|a) = 1$. This path probability distribution due to dynamical instability is studied in connection with information theory and action integral on the basis of the assumption that the different paths are uniquely differentiated by their actions defined for classical mechanical systems by

$$A_{ab}(k) = \int_{t_{ab}(k)} L_k(t) dt$$  

(3)

where $L_k(t)$ is the Lagrangian of the system at time $t$ along the path $k$. The average action between state $a$ and state $b$ can be given by

$$A_{ab} = \sum_{k=1}^{\nu} p_k(b|a) A_{ab}(k)$$  

(4)

For all stochastic process like Brownian motion[17], it can be proved[16] that the most probable paths are just the paths of least action. The probability of other paths decreases exponentially with increasing action.
In this work, we introduce another approach in order to study a more general situation where the systems under consideration moves from an initial cell \( a \) to different destinations \( b \) with a given travelling time, as shown in Figure 1(II). This “spacial uncertainty” and the “time uncertainty” studied in [16] are two aspects of the same dynamical instability. That is, for regular motion, these two uncertainties both disappear.

Now let us consider an ensemble of large \( N \) identical systems leaving the initial cell \( a \) in the initial phase volume \( A \) for some destinations in the phase volume \( B \) formed by the final phase points occupied by the systems. The travelling time is \( t_{ab} = t_b - t_a \) fixed for every trajectory and destination. After \( t_{ab} \), all the phase points occupied by the systems are found in the volume \( B \) partitioned into cells labelled by \( b \). We observe \( N_{kb} \) systems travelling along a path \( k_b \) leading to certain cell \( b \). A path probability can be defined by \( p_{k_b|a} = N_{kb}/N \) which is normalized by

\[
\sum_b \sum_{k_b=1}^{w_b} p_{k_b|a} = 1. \tag{5}
\]

where \( w_b \) is the number of possible paths from \( a \) to a given cell \( b \) of the volume \( B \). We always suppose each path is characterized by its action \( A_{k_b|a} \). Then an average action can be defined by

\[
A_a = \sum_b \sum_{k_b=1}^{w_b} p_{k_b|a} A_{k_b|a} \tag{6}
\]

The uncertainty concerning the choice of paths and final cells is measured by the following Shannon information

\[
H_{B|a} = -\sum_b \sum_{k_b=1}^{w_b} p_{k_b|a} \ln p_{k_b|a} \tag{7}
\]

which can be maximized under the constraints associated with Eq.(5) and Eq.(6) as follows

\[
\delta(H_{B|a} + \alpha \sum_b \sum_{k_b=1}^{w_b} p_{k_b|a} + \eta \sum_b \sum_{k_b=1}^{w_b} p_{k_b|a} A_{k_b|a}) = 0. \tag{8}
\]

This leads to

\[
p_{k_b|a} = \frac{1}{Z} \exp[-\eta A_{k_b|a}], \tag{9}
\]
where \( Z = \sum_{b}^{overB} \sum_{b}^{k} \exp[-\eta A_{b|a}] \). Putting Eq. (9) back into Eq. (7), we get

\[
H_{B|a} = \ln Z + \eta A_a = \ln Z - \eta \frac{\partial}{\partial \eta} \ln Z.
\]  

(10)

It is proved that[16] the distribution Eq. (9) is stable with respect to the fluctuation of action. It is also proved that if \( \eta \) is positive, Eq. (9) is a least action distribution, i.e., the most probable paths are just the paths of least action. On the contrary, if \( \eta \) is negative, then Eq. (9) is a most action distribution which means that the most probable paths maximize action. In any case, whatever the sign of the parameter \( \eta \), the most probable paths which maximize the path information always correspond to extremum or stationary action (\( \delta A_{b|a} = 0 \)). In other words, for instable dynamical process, the method of maximum information must be used in order to derive correct probability distribution just as the principle of stationary action must be used to derive the correct trajectories for regular dynamics.

In our previous work[16], Brownian motion was presented as an example of the case of \( \eta > 0 \). We would like to mention in passing that this model of Brownian motion allowed us to give a simple derivation of Fick law for particle diffusion and of Fourier law for heat conduction in solids[18] thanks to the distribution function Eq. (9).

4 Maximum entropy change

The question here is how to derive the invariant measures \( \mu_i \) with which the entropy \( S \) for dynamical systems is defined through Eq. (2). In what follows, we suppose that entropy changes when a system moves from the initial cell \( a \) to the final cell \( b \). The initial entropy of the systems at time \( t = 0 \) is given by Shannon formula:

\[
S_a = -\sum_{a} \mu_a \ln \mu_a
\]  

(11)

where \( \mu_a \) is the invariant measure of the systems in the initial phase volume \( A \) at \( t = 0 \) and the cell index \( a \) is summed over all the occupied cells in \( A \). After a period of time \( t_{ab} \), the system travelling along a path \( k_b \) is found in a cell \( b \) with probability measure \( \mu_{k_b}(a) \). Supposing the transition probability is independent of the distribution \( \mu_a \) of initial conditions, we have

\[
\mu_{k_b}(a) = \mu_a p_{k_b|a}.
\]  

(12)
The entropy of the system after \( t_{ab} \) should be defined by

\[
S_b = - \overline{\sum_a \sum_b \sum_{k_b} \mu_{k_b}(a) \ln \mu_{k_b}(a)}
\]

(13)

\[
= - \overline{\sum_a \mu_a \ln \mu_a} - \overline{\sum_a \sum_b \sum_{k_b} p_{k_b|a} \ln p_{k_b|a}}
\]

\[
= S_a + \sum_a \mu_a H_{B|a} = S_a + H_{B|A},
\]

where \( H_{B|A} \) is the average of the path information \( H_{k|a} \) over all the initial phase volume \( A \). So if \( H_{B|a} \) is maximized, \( H_{B|A} \) should also be maximized. The sums in the above equation must be over all the cells in the initial phase volume \( A \), in the final phase volume \( B \) (formed by all cells \( b \)) and over all the possible paths between \( A \) and \( B \).

Eq.(13) can be written as

\[
\Delta S = S_b - S_a = H_{B|A} = \langle \ln Z \rangle + \eta \langle A \rangle,
\]

(14)

where \( \langle \ln Z \rangle \) and \( \langle A \rangle \) are the averages of \( \ln Z \) and \( A_a \) on the volume \( A \). Eq.(14) is the main result of this work. It is obvious that the maximization of \( H_{B|A} \) means the maximization of the entropy change \( \Delta S \) of the dynamical process.

5 What about maximum entropy?

Maximum entropy change for dynamical systems does not exclude the possibility of maximum entropy. In fact, if the entropy change is maximized at any moment of an evolution with respect to different probability distributions, given the initial entropy \( S_a \), the entropy \( S_b \) of the final states must also be at maximum all the time with respect to the same distributions. So in order to derive correct probabilities or invariant measures, both entropy change and entropy can be maximized, depending on which of the two quantities is available as function of the probability distributions to be derived.

If the initial phase volume \( A \) and the final volume \( B \) represent equilibrium states, i.e., the dynamical process connects two Clausius entropies \( S_a \) and \( S_b \), then Boltzmann and Gibbs formula can be maximized to derive equilibrium probability distributions \( p_i \) of final states, as suggested by Jaynes principle.
This can be considered as a derivation of the maximum entropy method from the maximum path information which is nothing but an application of the action principle of classical mechanics.

6 Concluding remarks

A path information is defined in connection with different possible paths of dynamical system moving in its phase space from the initial cell towards different final cells. On the basis of the assumption that the paths are physically differentiated by their actions, we show that the maximum path information leads to a path probability distribution implying that the most probable paths are just the paths of stationary action. It is also shown that the average path information defined in this work is just the variation of the entropy during the dynamical process. Hence the principles of least action and of maximum path information suggest the maximum entropy change for dynamical systems. For given initial distribution, maximum entropy change means in fact the maximization of final entropy with respect to the same probability distributions.

We would like to mention that the intrinsic link between entropy and action tells us that the information theory and statistical mechanics do not need that entropy be an anthropomorphic quantity. Information and entropy are nothing but objective measures of dynamical uncertainty when the motion of physical systems become probabilistic. So maximum information and entropy is not merely an inference principle. It is a law of physics. This is the main conclusion of this paper.

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Figure 1: (I) The possible phase space paths \((k = 1, 2, ... w)\) for a system to go from the cell \(a\) to the cell \(b\) in time \(t_{ab}(k)\), each having a probability \(P_{ab}(k)\). If \(w\) is the number of all the possible paths, we have \(\sum_{k=1}^{w} P_{ab}(k) = 1\). (II) The possible phase space paths for a system to go from a given cell \(a\) to the different cells \(b\) of a partition of the final phase volume \(B\) during the time \(t_{ab}\), each having a probability \(p_{k_b|a}\). More than one paths from \(a\) to a given cell \(b\) are allowed so we may have \(k_b = 1, 2, ... w_b\) where \(w_b\) is the total number of paths from \(a\) to a cell \(b\).
Figure 1