

A Bayesian Perspective on Markovian Dynamics and the Fluctuation Theorem

Nathaniel Virgo

Max Planck Institute for Biogeochemistry, Jena, Germany; now at University of Tokyo, Japan

Abstract. One of E. T. Jaynes' most important achievements was to derive statistical mechanics from the maximum entropy (MaxEnt) method. I re-examine a relatively new result in statistical mechanics, the Evans-Searles fluctuation theorem, from a MaxEnt perspective. This is done in the belief that interpreting such results in Bayesian terms will lead to new advances in statistical physics.

The version of the fluctuation theorem that I will discuss applies to discrete, stochastic systems that begin in a non-equilibrium state and relax toward equilibrium. I will show that for such systems the fluctuation theorem can be seen as a consequence of the fact that the equilibrium distribution must obey the property of *detailed balance*. Although the principle of detailed balance applies only to equilibrium ensembles, it puts constraints on the form of non-equilibrium trajectories.

This will be made clear by taking a novel kind of Bayesian perspective, in which the equilibrium distribution is seen as a *prior* over the system's set of possible trajectories. Non-equilibrium ensembles are calculated from this prior using Bayes' theorem, with the initial conditions playing the role of the data. I will also comment on the implications of this perspective for the question of how to derive the second law.

Keywords: fluctuation theorem, non-equilibrium statistical mechanics, Bayesian perspective

PACS: 05.50.-a

INTRODUCTION

This paper presents a novel Bayesian perspective on statistical mechanics, with a particular focus on a relatively new result in non-equilibrium statistical mechanics known as the fluctuation theorem. (See [1, 2] for detailed overviews of this theorem and its applications.) The primary purpose of this paper is not to present new physical results, but to summarise several known results in the modern language of Bayesian probability theory. I hope that the insights gained will form the basis of new results in future work.

Early proofs of the fluctuation theorem were relatively complex, and applied only to various specific classes of system. A version of the fluctuation theorem was derived within Jaynes' MaxEnt framework by Dewar [3, 4]. Dewar's derivation in [4] is notable for its simplicity and generality: it follows in a line or two from a simple maximum entropy assumption. In this paper I will take a slightly different approach to deriving the fluctuation theorem from Bayesian principles. The derivation given below is of a similar level of simplicity to Dewar's, but relies on different assumptions.

DISCRETE SYSTEMS IN EQUILIBRIUM

We consider a physical system that can take on a discrete number of (microscopic) states. This system is assumed to be in contact with a heat bath of temperature T . The usual

formalism of statistical mechanics tells us that, at equilibrium, the probability of the system being in state i is given by

$$p_i = \frac{1}{Z} e^{-\beta u_i}, \quad (1)$$

where u_i is the energy of the system's i^{th} state, $\beta = 1/kT$ is the inverse temperature, and $Z = \sum_i e^{-\beta u_i}$ is a normalisation factor known as the partition function. Jaynes [5] showed that this can be extended to the case where a system can exchange any number of different conserved quantities with its environment, such as volume, particle number, electric charge and so on. If we let the value of the j^{th} such quantity in the system's i^{th} microstate be f_i^j then the equilibrium probability becomes

$$p_i = \frac{1}{Z} e^{-\sum_k \lambda_k f_i^k}, \quad (2)$$

The parameters λ_k are related to the intensive quantities of thermodynamics: if f_i^1 , f_i^2 and f_i^3 are the internal energy, volume and particle number of a given state, then $\lambda_1 = 1/T$, $\lambda_2 = p/T$ and $\lambda_3 = -\mu/T$, with T the system's temperature, p the pressure, and μ the chemical potential.

When the system is in equilibrium with its environment, the quantities λ_k can be interpreted as the temperature, pressure, etc. of the system, and they will be equal to the corresponding quantities for the environment. Later on we will drop the assumption that the system is in an equilibrium state. However, we will assume that its environment (the heat bath) remains in equilibrium at all times, and that its intensive variables do not change. From now on we will therefore think of the values λ_k as being strictly properties of the system's environment, rather the properties of the system itself.

Below we will make use of Einstein's inversion of Boltzmann's formula $S = \log W$ for the entropy, which is given by $p_i \propto e^{S_i}$, where we have set Boltzmann's constant to 1 for convenience. Here, S_i is the entropy of the heat bath (in natural units) when the system is known to be in state i .

The probabilities p_i are considered constant over time. We now wish to consider the behaviour of the system over time. We begin by considering the time-dependent behaviour of the equilibrium state. To do this we must make some additional assumptions and introduce some new notation. We will assume that time moves forward in discrete steps. Let a "trajectory" be represented by a function $x(t)$, indicating the state of the system at each time step t . This allows us to write $p(x(t) = i)$ for the probability of the system being in state i at time t . For the equilibrium distribution, we have that $p(x(t) = i) = p_i$ for every i , with p_i as defined in Equation 2. $x(t)$ can be thought of as a collection of random variables — one for each value of t — that are jointly distributed.

A common assumption in statistical mechanics is that the dynamics are Markovian. That is, $x(t-1)$ and $x(t+1)$ are conditionally independent given $x(t)$, for every t . It is worth noting that, except in the limiting case of deterministic behaviour, this assumption entails "throwing away" some information at every time step.

We may consider the system and its environment together to make up a single isolated system, whose combined dynamics are both deterministic and reversible. From a Bayesian perspective, the stochastic dynamics arise because we choose to ignore some

information about dynamics of the heat bath. We now show that the Markovian assumption arises naturally if we throw away not just some but all information about the heat bath's dynamics. Conceptually, to do this we must at every time step replace the probability distribution over the environment's microscopic states with a maximum entropy distribution. This is similar to the procedure described in [6], where the entropy of an isolated system is repeatedly re-maximised subject to constraints formed by its macroscopic state. In our case the isolated system consists of both the system of interest and the heat bath, and the role that the macroscopic state plays in Jaynes' exposition is in our case played by x , the microscopic state of the system of interest alone.

If we let the heat bath's microscopic state be denoted y , the Hamiltonian assumption of deterministic, reversible dynamics amounts to saying that the combined state at the next time step, $(xy)(t)$, is a one-to-one function of $(xy)(t-1)$, the combined state at the current time step. Remaximisation of entropy entails replacing the joint probability distribution $p((xy)(t) = ij)$ with one that can be factorised as $p(x(t) = i)p(y(t) = j | x(t) = i)$. That is, we explicitly remove any dependence of $y(t)$ on anything other than $x(t)$ after every time step. This amounts to assuming that the (microscopic) internal dynamics of the heat bath y are irrelevant for predicting the future (microscopic) states of the system x . As a result of this approximation, $x(t+1)$ cannot depend on the system's state at times prior to t . Whether it is a good approximation or not will depend on the circumstances, and in particular on where we choose to draw the line between the system and its environment.

In addition to this Markovian assumption, the equilibrium distributions of physical systems must obey the condition of *detailed balance*:

$$\frac{p_{i \rightarrow j}}{p_{j' \rightarrow i'}} = \frac{p_j}{p_i}. \quad (3)$$

The notation $p_{i \rightarrow j}$ is shorthand for $p(x(t+1) = j | x(t) = i)$, and is to be thought of as the probability of the system transitioning from state i to state j in a single time step. The states i' and j' represent the "time-reversal" of i and j , formed by reversing the velocity of every particle. In the equilibrium ensembles usually considered, $p_{i'}$ is always equal to p_i . Equation 3 arises from the fact that x must evolve according to effective stochastic dynamics that are invariant with respect to this time-reversal operation.

The Non-Equilibrium Case

The property of detailed balance does not apply to non-equilibrium ensembles, in the following sense: consider an ensemble of systems that at time 0 are in some distribution other than the equilibrium one. Let the probability of the i^{th} state at time t according to this ensemble be denoted $q_i(t)$. (In more Bayesian notation we can write $q_i(t) = p(x(t) = i | Q)$, where Q is to be interpreted as some additional information about the system's state at time t . See below for more details.) Now it cannot be the case that $\frac{p_{i \rightarrow j}}{p_{j' \rightarrow i'}} = \frac{q_j(t)}{q_i(t)}$ for every i and j unless every $q_i(t) = p_i$.

However, the conditional probabilities $p_{i \rightarrow j} = p(x(t+1) = j | x(t) = i)$ do not depend upon whether we are considering an equilibrium or a non-equilibrium ensemble. This

is due to the Markovian assumption: the initial conditions can only affect the state at a time t through their effect on the state at intermediate times. Equation 3 therefore *does* hold for non-equilibrium trajectories, as long as we interpret p_i and p_j as the unconditional *equilibrium* probabilities, and not as the time-dependent probabilities of the non-equilibrium ensemble.

From Einstein's inversion of Boltzmann's formula we have that

$$\frac{p_{i \rightarrow j}}{p_{j' \rightarrow i'}} = e^{S_j - S_i}, \quad (4)$$

which again must hold regardless of whether the trajectory resulted from non-equilibrium initial conditions or simply as a fluctuation from the equilibrium state. This is, essentially, the fluctuation theorem. Note that S_j and S_i are the entropy of the environment when the system is in a given state, and we assume the environment is always in thermal equilibrium. There is therefore no difficulty in interpreting $S_j - S_i$ as a change in thermodynamic entropy, even if the system is very far from equilibrium.

This argument is essentially a stripped-down version of the one given by Onsager [7], without the additional near-equilibrium assumptions that lead to linear macroscopic behaviour. The novel aspect of the present work will appear below, when we re-express the argument in terms of Bayesian probability theory.

Non-equilibrium ensembles as Bayesian posteriors

In this section we present a slightly different perspective on the above result. To do so we make use of a formalism for probability theory developed by Cox [8] in which probabilities are seen as applying not to random variables but to statements of logic. See Jaynes' book [9] for a detailed explanation of this formalism and its applications.

We first consider the set of equilibrium trajectories. We will denote a trajectory from time 0 to time n by $x_0 x_1 \dots x_n$, and we will let Γ represent the actual trajectory taken in a given experiment. The probability of a given trajectory may be written

$$\begin{aligned} p_{x_0 x_1 \dots x_n} &= p(\Gamma = x_0 x_1 \dots x_n) \\ &= p(x(0) = x_0 \wedge x(1) = x_1 \wedge \dots \wedge x(n) = x_n). \end{aligned} \quad (5)$$

By the Markovian assumption,

$$p_{x_0 x_1 \dots x_n} = p_{x_0} \prod_{t=0}^{n-1} p_{x_t \rightarrow x_{t+1}}. \quad (6)$$

We now wish to calculate the probability distribution over trajectories for a system that is known to begin in state i , i.e. we are given the boundary conditions $x(0) = i$. We will denote these probabilities $q_{x_0 x_1 \dots x_n}$. They are given by

$$q_{x_0 x_1 \dots x_n} = \prod_{t=0}^{n-1} p_{x_t \rightarrow x_{t+1}} \quad \text{if } x_0 = i, \quad \text{and 0 otherwise.} \quad (7)$$

But the same result is obtained by calculating the conditional probability

$$p(\Gamma = x_0x_1 \dots x_n | x(0) = i), \quad (8)$$

which may be found using Bayes' theorem. We may therefore think of $q_{x_0x_1 \dots x_n}$ as simply a notational shorthand for this conditional probability. From this perspective, we may view the distribution $p_{x_0x_1 \dots x_n} = p(\Gamma = x_0x_1 \dots x_n)$ not as the dynamics of a system in equilibrium but as a Bayesian prior over the space of all trajectories, which we may update to a posterior using Bayes' theorem if we receive some extra information (or "data") about the initial conditions.

This may be extended to the more general case where the initial conditions are given by a probability distribution q_i^0 , rather than simply $x(0) = i$. In this case we introduce a statement Q such that

$$p(x(0) = i | Q) = q_i^0 \quad \text{and} \quad (9)$$

$$p(x(t) = j | x(0) = i \wedge Q) = p(x(t) = j | x(0) = i) \quad (10)$$

for all i, j and t . From this one may use only the rules of probability theory to obtain

$$p(\Gamma = x_0x_1 \dots x_n | Q) = q_{x_0}^0 \prod_{t=0}^{n-1} p_{x_t \rightarrow x_{t+1}}. \quad (11)$$

It might seem odd that we have asserted the existence of a statement Q without explicitly writing an expression for it. The point is that the result will hold for any Q for which Equations 9 and 10 hold; we may think of these relationships as defining Q .

The constraint given by Equation 10 tells us that Q does not give us any information about $x(t)$ beyond the information it gives about $x(0)$. Without it, Q cannot be said to be information about the initial conditions — instead it is some more general information about the trajectory as a whole — and Equation 11 cannot be derived.

A Toy Example

The above ideas can be illustrated by Monte Carlo sampling of a simple "toy model." We consider a system with a countable number of states (numbered $1, 2, \dots$), such that the i^{th} state has energy E equal to i . The equilibrium probability of being in state i is thus proportional to $e^{-\beta i}$, where β is the inverse temperature of a heat bath to which we suppose the system is connected. We set $\beta = 1$ for simplicity. In this case the equilibrium distribution can be found analytically, to give $p_i = (e - 1)e^{-i}$, and an expected energy of $e/(e - 1) \approx 1.58$. We must now choose probabilities for the state transitions. These must obey the detailed balance relation $p_{i \rightarrow j}/p_{j \rightarrow i} = p_j/p_i$. We choose $p_{i \rightarrow i+1} = e^{-\beta}$ and $p_{i+1 \rightarrow i} = \frac{1}{2}$, implying that the system can exchange at most one unit of energy with the heat bath in a given time step. (For the "ground state" $i = 1$, there is no probability to transition to a lower state, just the probability $e^{-\beta}$ of transitioning to state 2.) These probabilities can be derived by applying the Metropolis algorithm, but here we conceptualise them as defining the system's dynamical behaviour, rather than as a way to numerically approximate the equilibrium distribution.

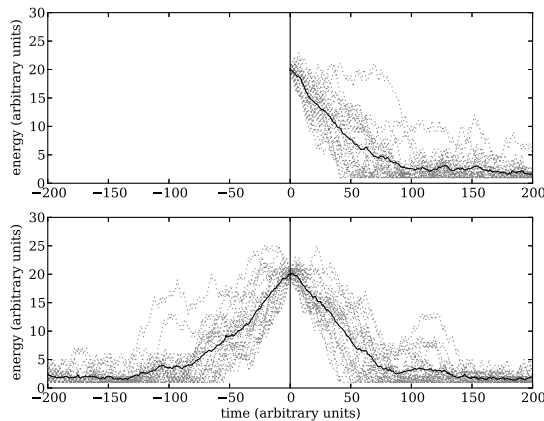


FIGURE 1. Plot showing the dynamics of a simple toy system, demonstrating that a system’s behaviour does not depend on whether it reached its present state through being initialised that way or via a fluctuation. The top image was obtained by repeatedly starting the system in state $E = 20$ at time 0, and iterating it stochastically as described in the text. 20 such trajectories are shown as grey dotted lines, and their mean behaviour is shown as a black solid line. The bottom image was obtained by starting the system in state $E = 1$ and iterating it for around 1.2×10^8 time steps. Occasionally the system fluctuates into the state $E = 20$, and 20 such trajectories were chosen at random and aligned to make the figure. The differences between the top plot and the right-hand half of the bottom plot are only due to stochasticity, and with a greater number of trials they will converge to the same overall behaviour.

Figure 1 shows samplings from the trajectories of this system, taken in two different ways. In the first plot we repeatedly start the system in the atypical state $i = 20$ and plot its dynamics over time as it relaxes back toward the equilibrium distribution centred on $E = 1.58$. In the second plot we instead start the system in its most probable state ($i = 1$) and iterate it for a very large number of time steps. Occasionally it fluctuates into the state where its energy equals 20, and we plot a selection of these. (Every time the system reaches state 20, we randomly choose whether to include it in the plot, with probability 0.1. This is to avoid correlations caused by the fact that the system often enters this state several times in quick succession, resulting in very similar trajectories.)

That the two plots look similar is not surprising. Because of the Markov property, the system’s past behaviour has no effect on its future behaviour, and so the expected behaviour of trajectories selected according to the two methods must be the same. The method used to plot the second figure can be thought of as “direct sampling” from the distribution of possible trajectories. This illustrates our point that computing a stochastic system’s behaviour from its initial conditions is equivalent to performing Bayesian inference using the equilibrium distribution as the prior and the initial state as the data.

THE ARROW OF TIME

Figure 1 also demonstrates another interesting point, to do with Boltzmann’s paradox. In the top plot, the energy starts out with a value of 20, and tends to decrease until it fluctuates around 1.58, when the total entropy is maximised. But in the lower plot, we see the energy increasing from around its equilibrium value, up to around 20. This means

that the total entropy decreases until time 0, and then increases again. This should not be surprising, because the stochastic dynamics of system in question are time reversal invariant.

Boltzmann's paradox is the name given to the puzzling fact that the second law of thermodynamics seems to impose a direction on time (i.e. the entropy increases in the direction of the future and decreases toward the past), while the underlying microscopic laws of physics are invariant under time reversal. The puzzle is that, in our everyday macroscopic experience, we often observe systems that are out of equilibrium. We expect such systems' entropy to be higher in the future, but we equally expect it to have been lower in the past. A boulder halfway up a mountainside did not fluctuate there due to thermal motion, but quite likely rolled there from an even higher position. Boltzmann realised after several failed attempts that the time-dependent second law could not be derived from the time-invariant microscopic laws alone; some additional assumption is always required. An interesting discussion of this issue can be found in [10].

In the Bayesian picture presented here, the resolution to this has to do with information, and specifically our information about the system and the world it interacts with. Figure 1 essentially tells us what we should expect if *all* we know about the system are its energy state, the fact that it is in contact with a heat bath with $\beta = 1$, and the fact that it was in a particular atypical state at a particular time. If this were really all the information we had about a physical system, it would be quite rational to conclude that it must have reached this state through a fluctuation. It would be just as reasonable to expect that the path it had taken to reach the non-equilibrium state would be a reverse of the path it will take to decay back to equilibrium in the future.

However, in our everyday experience, we typically have a lot more information than that: we know that we live in a far-from-equilibrium world, and we know that any given system is likely to have interacted with other systems in the past. This allows us to reject the unlikely hypothesis of a thermal fluctuation and look for other possible causes of the far from equilibrium state. In a world with plate tectonics and glaciers we have no need to consider thermal fluctuations as an explanation for the boulder on the mountainside.

We now tie this idea into several previous explanations of the arrow of time. Jaynes [6] presents an argument that is closely related to the one presented here. A clear exposition of Jaynes' argument is given by Dewar in [11]. Jaynes' argument hinges on the fact that we, as experimenters, can directly manipulate the initial conditions of an experiment but not the final ones. If we take this as axiomatic then it is clear that the left-hand half of Figure 1 corresponds to an unphysical situation, in which the final conditions of an experiment have been manipulated, rather than the initial ones.

Evans and Searles [2] present a derivation of the second law from the fluctuation theorem. This argument relies on an assumption of "causality", essentially the ability of an intervention in a system to affect its future trajectory, but not its past. This assumption is somewhat similar to Jaynes'. Both of these explanations are elegant, but both leave a question unanswered: what is the origin of this condition of causality?

Perhaps one answer to this could come from the "cosmological" argument for the second law, a form of which was originally proposed by Boltzmann [12], and which is nowadays widely accepted. The modern version of this idea states that the second law arises because the universe began in a very low entropy state immediately after the big bang. Effectively, the universe as a whole resembles the right-hand side of the plots in

Figure 1, in that it has low-entropy boundary conditions on one side and is unconstrained on the other. On this view, both Jaynes' observation (that experimenters can affect initial but not final conditions), and the "causality" condition, must be consequences of the boundary conditions that apply to the universe as a whole. Proving that these things follow from the cosmological boundary conditions is an interesting task for future work.

CONCLUSION AND OUTLOOK

We have made a small contribution to the task of expressing non-equilibrium statistical mechanics within a rigorous Bayesian framework. Within this framework, the equilibrium distribution takes on a new meaning: it now represents a Bayesian prior over the set of possible trajectories that the system may take over time. We consider this prior to represent the state of knowledge of someone who knows the intensive thermodynamic properties of the system's environment but has no extra knowledge about the system's state. If we do have some extra information about the system's initial conditions, this prior-over-trajectories can be updated to a posterior via an application of Bayes' theorem. This gives the same result as the usual calculation of a non-equilibrium ensemble.

The fluctuation theorem of Evans and Searles is a property of this posterior distribution. We have shown that it can be seen as arising from the fact that the prior distribution has the property of detailed balance. It is interesting to note that while the property of detailed balance in equilibrium distributions was known by Boltzmann, the fluctuation theorem was not discovered until the 1990s, around 100 years later. The latter can be easily derived from the former within this Bayesian framework, and this suggests that this Bayesian perspective could be a useful tool to derive new results in future work.

Finally, we have touched upon the issue of the arrow of time. The Bayesian perspective adds some clarity to the question of how some of the various approaches to deriving the second law of thermodynamics relate to one another.

REFERENCES

1. E. M. Sevcik, R. Prabhakar, S. R. Williams, and D. J. Searles, *Annual Review of Physical Chemistry* **59**, 603–633 (2008).
2. D. J. Evans, and D. J. Searles, *Advances in Physics* **51**, 1529–1585 (2002).
3. R. C. Dewar, *Journal of Physics A: Mathematical and General* **36**, 631–641 (2003).
4. R. C. Dewar, *Journal of Physics A: Mathematical and General* **38**, 371–381 (2005a).
5. E. Jaynes, *Phys. Rev.* **106**, 620–630 (1957).
6. E. Jaynes, *Am. J. Phys* **33**, 391–398 (1965).
7. L. Onsager, *Phys. Rev.* **37**, 405–426 (1931).
8. R. T. Cox, *American Journal of Physics* **14** (1946), reprinted in Shafer, G. and Pearl, J. (eds) *Readings in Uncertain Reasoning*. Morgan Kaufman Publishers, 1990.
9. E. Jaynes, *Probability Theory: the Logic of Science*, Cambridge University Press, Cambridge, 2003.
10. H. Price, *Time's Arrow and Archimedes' Point: New Directions for the Physics of Time*, Oxford University Press, New York ; Oxford, 1996.
11. R. C. Dewar, "Maximum Entropy Production and Non-Equilibrium Statistical Mechanics," in *Non-equilibrium Thermodynamics and the Production of Entropy*, edited by A. Kleidon, and R. D. Lorenz, *Understanding Complex Systems*, Springer, Berlin, 2005, pp. 41–53.
12. L. Boltzmann, *Vorlesungen über Gastheorie: Vol I*, J. A. Barth, Leipzig, 1896, translated by S. G. Brush, *Lectures on Gas Theory*, Berkeley: University of California Press, 1964.