The Backwards Arrow of Time of the Coherently Bayesian Statistical Mechanic

Cosma Rohilla Shalizi  

Center for the Study of Complex Systems, 4485 Randall Laboratory, University of Michigan, Ann Arbor, MI 48109 USA

Many physicists think that the maximum entropy formalism is a straightforward application of Bayesian statistical ideas to statistical mechanics. Some even say that statistical mechanics is just the general Bayesian logic of inductive inference applied to large mechanical systems. This approach identifies thermodynamic entropy with the information-theoretic uncertainty of an (ideal) observer’s subjective distribution over a system’s microstates. In this brief note, I show that this postulate, plus the standard Bayesian procedure for updating probabilities, implies that the entropy of a classical system is monotonically non-increasing on the average — the Bayesian statistical mechanic’s arrow of time points backwards. Avoiding this unphysical conclusion requires rejecting the ordinary equations of motion, or practicing an incoherent form of statistical inference, or rejecting the identification of uncertainty and thermodynamic entropy.

Recent years have seen renewed interest in connections between physics and statistics [1]. Of particular interest, naturally, has been the connection between statistical mechanics and statistical inference. The subjectivist approach to statistical mechanics, ably advocated in recent times by Jaynes [2] and his school, holds that probabilities represent degrees of belief; specifically, the probability of a microstate is the degree to which an ideal observer should believe the system is in that state, given the evidence available, and the entropy of the system is that observer’s uncertainty as to the microstate. The theory governing the coherent use of subjective probabilities is called Bayesian statistics [2]. Jaynes, in particular, claimed that statistical mechanics is just an application of the general logic of Bayesian inference. The validity of statistical mechanics would then be independent of such tricky dynamical properties as ergodicity, mixing, etc., which on other interpretations are vital. For subjectivists, the intensive study of the ergodic properties of mechanical systems is simply time wasted.

While controversial [2], the Bayesian vision of statistical mechanics is powerful and appealing. However, it has a flaw which has not been pointed out before. The second law says that the entropy of a closed system is non-decreasing; this provides the arrow of time. In [1] I prove that, equating thermodynamic entropy with subjective uncertainty, ordinary Bayesian inference implies that entropy is non-increasing over time, at least on average and sometimes strictly. ([1] investigates the long-run behavior of the distribution under Bayesian updating; it is ancillary to the main line of argument.) This is completely unphysical, so [1] examines the proof’s assumptions. There are strong arguments that any coherent use of subjective probabilities must employ Bayesian updating. In any case, replacing it by repeated applying the maximum entropy principle still reverses the arrow of time. This forces a choice between inconsistent, ad hoc rules of statistical inference, or abandoning the equation of physical entropy with uncertainty.

This rest of this introduction fixes notation, following [2, 3, 4], and makes explicit some innocent assumptions. Start with a classical mechanical system with a phase space \( \Gamma \); write \( x \) for a point in this phase space. \( F \) is a distribution on \( \Gamma \), representing an (ideal) observer’s uncertainty about the microscopic state \( s \). For simplicity, assume this distribution has a density \( f \) (i.e., is absolutely continuous with respect to Lebesgue measure on \( \Gamma \)). Denote expectation by angle brackets, so the mean of \( M \) is \( \langle M \rangle \); subscripts will specify the distribution used in the expectation when necessary, i.e. \( \langle M \rangle_F \) is the mean of \( M \) under distribution \( F \). \( \langle M | N \rangle \) is the expectation of \( M \) conditional on \( N \).

The system’s equations of motion lead to a discrete-time evolution operator \( T \) on \( \Gamma \), which I will assume is non-singular. (Everything still works in continuous time, but needs more symbols.) By a slight abuse of notation, \( T \) also denotes the induced Frobenius-Perron operator taking distributions on \( \Gamma \) into new distributions on \( \Gamma \). The specification of \( T \) also induces an evolution operator for observables, the Koopman operator \( U \), such that \( U \phi(x) = \phi(T(x)) \) for any sufficiently well-behaved \( (L^\infty) \) function \( \phi \). From this definition, it can be seen that \( \langle U \phi | F \rangle = \langle \phi | T_F \rangle \). (The difference between the Frobenius-Perron and Koopman operators is like that between the Schrödinger and Heisenberg pictures, respectively.)

There is, in addition to the microscopic degrees of freedom, a set of macroscopic degrees of freedom, collectively \( M \). These observables depend only on the present microscopic state, though possibly noisily, through some observation density \( p(M = m | X = x) \).

Write \( F_0 \) for the initial distribution, and \( F_t \) for the distribution at time \( t \). The distribution \( F_0 \) may be derived via a maximum-entropy procedure, starting from an initial observation \( M(0) = m_0 \) [2]. However, it re-

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*Electronic address: cshalizi@umich.edu*
ally doesn’t matter where \( F_0 \) comes from, or what form it takes. Finally, write \( H[F] \) for the Shannon entropy of the distribution \( F \), i.e.,

\[
H[F] \equiv - \int_{\Gamma} f(x) \log f(x) dx
\]

The information content of a random variable \( X \) is defined to be the entropy of its distribution function, which for convenience will also be written \( H[X] \); it should always be clear which is meant. Conditional information content, \( H[X|Y = y] \), is the entropy of the conditional distribution.

I. DERIVATION OF THE BACKWARDS ARROW

So far, I have either been fixing notation, or making assumptions which are common to all approaches to statistical mechanics, and so presumably innocuous. I now make three explicit and substantive assumptions.

I The evolution operator \( T \) is invertible.

II The probability distribution over microstates gets updated by the usual application of Bayes’s rule, \( p(X = x | Y = y) = p(Y = y | X = x) p(X = x) / p(Y = y) \).

III The thermodynamic entropy at time \( t \), \( S_t \), is equal to \( H[F_t] \).

These assumptions reverse the arrow of time, i.e., they make entropy non-increasing.

Begin with the initial distribution over microstates, \( F_0 \). After one time step, this is transformed to a new distribution, \( T F_0 \). From a Bayesian perspective, this does not represent a change in our knowledge of the system, merely keeping our predictions up to date. (Rather than updating the distribution, we could use the Koopman operator to update observables.) It is a well-known consequence of assumption I that \( H[T F_0] = H[F_0] \), i.e., that conservative dynamics are entropy-preserving [Theorem 9.3.1]. However, we now make a new measurement of the macroscopic observable \( M \), getting the value \( m_1 \). Then, via assumption II Bayes’s rule gives us a new distribution:

\[
f_1(x) = \frac{p(m_1 | x) T f_0(x)}{\int_{\Gamma} p(m_1 | x) T f_0(x) dx}
\]

Now, \( f_1(x) \) is simply the density of \( X_1 \), conditional on \( M_1 = m_1 \). So \( H[F_1] = H[X_1 | M_1 = m_1] \). An elementary inequality of information theory [I] tells us that “conditioning reduces entropy”; specifically, \( H[X|M] = \langle H[X] | M = m \rangle \leq H[X] \), with equality if and only if \( X \) and \( M \) are statistically independent. Using assumption III to identify the thermodynamic entropy \( S_t \) and the Shannon information \( H[F_t] \),

\[
\langle S_1 \rangle = \langle H[F_1] \rangle \leq H[F_0] = S_0
\]

Thus, unless the macroscopic observable is in fact merely noise, the entropy decreases on average. While there may be values of \( m \) which are so uninformative they increase an observer’s uncertainty about the microspscopic state, on average every observation helps narrow that uncertainty.

A stronger result follows from the common idealization that observables are deterministic functions of microscopic state, \( M(x) = m \). In this case, \( p(m | x) \) is either 0 or 1, depending on whether \( M(x) = m_1 \) or not. Thus \( f_1(x) = T f_0(x) \chi_{M^{-1}(m_1)}(x) / T F_0(M^{-1}(m_1)) \), i.e., the truncation of \( T F_0 \) to the part of \( \Gamma \) compatible with the macroscopic observation. Unless \( M^{-1}(m_1) \) includes the entire support of \( T F_0 \), \( F_1 \) is a more concentrated measure than \( T F_0 \) or \( F_0 \), and so the entropy has strictly decreased, and not just on average.\(^1\)

Under repeated measurements, the entropy is non-increasing, either on average or strictly, depending on whether the measurements are noisy or not. (Entropy is constant between observations.) In the case of discrete-valued deterministic measurements, if the measurement partition is “generating” \( \mathcal{G} \), then the volume of \( \Gamma \) compatible with a sequence of measurements shrinks towards zero, and so the uncertainty, as measured by the Shannon information, tends to \(-\infty\). This is not necessarily the case if the measurement partition is not generating.

Note that I required nothing of the dynamics other than assumption II invertibility. In particular, I did not need chaos, ergodicity, mixing, etc., either at the microscopic or macroscopic level. Thermodynamic equilibrium or its absence is also irrelevant.

A. Long-Run Behavior of \( H[F_t] \)

Describing the long-run behavior of \( H[F_t] \) requires explicit use of measure-theoretic probability [II], and what’s called “Doob’s martingale”. As a measurable space, \( \Gamma \) comes with a \( \sigma \)-algebra of measurable sets \( \mathcal{G} \). Let \( G \) be any set in \( \mathcal{G} \). Then \( 1_G(X) \) is a random variable, indicating whether or not \( X \in G \), and \( \langle 1_G \rangle_{F_0} = F(G) \), the probability of the set \( G \) under distribution \( F_0 \). Let \( M_t = \sigma(M_1, \ldots, M_t) \), the smallest \( \sigma \)-algebra with respect to which all the observables up to \( M_t \) are measurable, and examine \( \langle 1_G | M_t \rangle_{F_0} \), the conditional expectation of the indicator variable for \( G \). Clearly, \( \langle 1_G | M_t \rangle_{F_0} = \langle 1_G \rangle_{F_t} = F_t(G) \). \( F_t(G) \) is a martingale and converges almost surely and in mean square to a random variable \( F_\infty(G) \), which is the conditional expectation of \( 1_G \) with respect to \( M_\infty \), the smallest \( \sigma \)-algebra containing all the \( M_t \) [II, §6.6]. Thus, the conditional measures \( F_t \) converge weakly on a limit \( F_\infty \) [II, §7.1]. Thus, the entropy of \( H[F_t] \) also

\(^1\) The most important case where supp \( T F_0 \subseteq M^{-1}(m_1) \) is when \( M \) is a constant of the motion, e.g., total energy for a Hamiltonian system. Entropy is then constant after the first measurement, even if the system begins arbitrarily far from equilibrium.
converges on a limiting value. If \( \mathcal{M}_\infty = \mathcal{G} \), as in the generating partition case, then, for any set \( G \), \( F_\infty(G) = 0 \) or \( = 1 \), and \( H[F_\infty] = -\infty \). If \( \mathcal{M}_\infty \subset \mathcal{G} \), then the conditional distributions converge weakly on a distribution with a finite entropy.\(^2\)

A somewhat more refined result is possible if we assume that the asymptotic equipartition property of information theory holds (i.e., that the Shannon-Macmillan-Breiman theorem applies). This leads to estimates of the asymptotic growth rates for likelihoods, and so for posterior probabilities in Bayes’s rule.

Suppose that the following limits exist for every \( x, y \in \Gamma \):

\[
\begin{align*}
    h(x) &\equiv \lim_{n \to \infty} \frac{1}{n} H[M_n | M_{n-1}, M_{n-2} \ldots M_1, X_0 = x] \\
    d(x, y) &\equiv \lim_{n \to \infty} \frac{1}{n} \int d^n m \ p(m^n_1 | x) \log p(m^n_1 | x) \\
    p(m^n_1 | x) &\text{ abbreviates } p(M_1 = m_1, M_2 = m_2, \ldots M_n = m_n | X_0 = x).
\end{align*}
\]

where \( p(m^n_1 | x) \) abbreviates \( p(M_1 = m_1, M_2 = m_2, \ldots M_n = m_n | X_0 = x) \). The quantity \( h(x) \) is the macroscopic entropy rate at \( x \) (not to be confused with the microscop ic rate of entropy production \(^{11}\)). \( d(x, y) \) is the macroscopic relative entropy rate, or Kullback-Leibler divergence rate, between \( x \) and \( y \). Note that \( d(x, y) \geq 0 \), and that \( d(x, y) = 0 \) if and only if \( p(M_n = m_n | M_{n-1} = m_{n-1}, X_0 = y) \) and \( p(M_n = m_n | M_{n-1} = m_{n-1}, X_0 = x) \) converge for almost all \( m^n_1 \) \(^{11}\). Further assume that the asymptotic equipartition property \(^{11}\) holds, so that, if \( X_0 = y \), then for \( F_0 \)-almost-all \( x \)

\[
\lim_{n \to \infty} \frac{1}{n} \log p(m^n_1 | x) = h(y) + d(x, y) \tag{7}
\]

almost surely. An immediate corollary of Eq. \(^{9}\) is that

\[
\log p(m^n_1 | x) = -nh(y) - nd(x, y) + g(x, y, m^n_1) \tag{8}
\]

where \( g \) is a random quantity which is \( o(n) \) almost surely.

Write Bayes’s rule with \( n \) observations in logarithmic form, and substitute in Eq. \(^{10}\) (assuming \( f_0(x) > 0 \)):

\[
\begin{align*}
    \log \frac{f_n(x)}{f_0(x)} &\equiv \log p(m^n_1 | x) - \log p(m^n_1 | x) | F_0 \\
    &\equiv -nh(y) - nd(x, y) + g(x, y, m^n_1) \\
    &- \log \left( \frac{\mathbb{E}[e^{-nh(y) - nd(x, y) + g(x, y, m^n_1)}]}{F_0} \right)
\end{align*}
\]

\[
\begin{align*}
\gamma &\equiv -nh(y) - nd(x, y) + g(x, y, m^n_1) \tag{11} \\
\gamma &\equiv -nd(x, y) + g(x, y, m^n_1) - \gamma(y, m^n_1) \\
\gamma &\equiv -\mathbb{E} \left[ e^{-nd(x, y) + g(x, y, m^n_1)} \right] \\
\gamma &\equiv -\mathbb{E} \left[ e^{-nd(x, y)} \right] \\
\gamma &\equiv -\mathbb{E} \left[ e^{-nd(x, y)} \right] \\
\gamma &\equiv -\mathbb{E} \left( e^{-nd(x, y)} \right) \\
\gamma &\equiv -\mathbb{E} \left( e^{-nd(x, y)} \right)
\end{align*}
\]

The last line defines \( d(x, y) \), and \( \| \phi(x) \|_{F_0} = \left( \| \phi(x) \|_{F_0} \right)^{1/n} \) is the \( L^n \) norm of the function \( \phi \) with respect to the measure \( F_0 \). The latter is non-decreasing in \( n \), and its limit is the essential supremum of the function. That is, \( \| e^{-d(x, y)} \|_{F_0} \) is the smallest \( u \) such that \( u \geq e^{-d(x, y)} \) for all \( x \), except on a set of \( F_0 \)-probability zero. It follows that \( d_\infty(y) \) is the essential infimum of \( d(x, y) \), and so \( d_\infty(y) \leq d(x, y) \) everywhere except on a set of \( F_0 \)-probability zero. Since \( d(x, y) \geq 0 \), we can be sure that \( d_\infty(y) \) is at least zero. Since \( d(y, y) = 0 \), if \( f_0 \) is positive in every sufficiently small neighborhood of \( y \), we will have \( d_\infty(y) = 0 \). Since the procedures used to construct prior distributions for statistical mechanics generally give non-vanishing weight to all physically accessible regions of the phase space, this last assumption is reasonable, and so set \( d_\infty(y) = 0 \).

Substituting back in to Eq. \(^{12}\)

\[
\begin{align*}
\log \frac{f_n(x)}{f_0(x)} &\equiv -nd(x, y) + \gamma(y, x, m^n_1) + \gamma(\eta(x, y, m^n_1)) \\
&\equiv n \left( d(x, y) - d(x, y) \right) + \gamma(y, x, m^n_1) \\
&\equiv n \left( d(x, y) - d(x, y) \right) + \gamma(y, x, m^n_1)
\end{align*}
\]

Taking the limit as \( n \to \infty \),

\[
\lim_{n \to \infty} \frac{1}{n} \log \frac{f_n(x)}{f_0(x)} = d_\infty(y) - d(x, y) \tag{17} \\
= d(x, y) \tag{18}
\]

Asymptotically, therefore, \( f_n(x) \) shrinks exponentially fast towards zero, unless \( d(x, y) = 0 \). Setting \( D(y) = \{ x | d(x, y) = 0 \} \), we see that \( F_\infty(D(y)) = 1 \), and so \( H[F_\infty] \) is at most the logarithm of the volume of \( D(y) \).

II. WAYS TO AVOID THIS RESULT

Since, in reality, thermodynamic entropy is monotonically non-decreasing, at least one of the assumptions leading to Eq. \(^{12}\) must be wrong.

\(^2\) By Eq. \(^{3}\) the sequence \( H[F_i] \) forms a supermartingale with respect to the filtration induced by the macro-variables \( M_t \), but the conditions needed to directly apply martingale convergence theorems, such as \( \langle |H[F_i]| \rangle < \infty \), do not necessarily hold.
A. Assumption II Invertible Dynamics

Denying assumption II “has all the advantages of theft over honest toil” [12]. The problem of the foundations of statistical mechanics is precisely that of deriving macroscopic irreversibility from microscopically-reversible dynamics, and the point of the Bayesian approach was to do so with making detailed assumptions about those dynamics. That said, crime may not pay; the conditions needed to get \( H[TF] \geq H[F] \) impose highly non-trivial restrictions on the dynamics [13]. Not only are conservative Hamiltonian dynamics ruled out, but so is any system of ordinary differential equations. What is really needed is that \( H[TF|M] \geq H[F] \), and it is hard to see why the microscopic dynamics should always produce more than enough entropy to off-set the information provided by whichever macroscopic observables we happen to choose. But without such cancellation, watching a pot closely enough will keep it from boiling.

B. Assumption III Bayesian Updating

Explicitly or not, most advocates of Bayesian statistical mechanics reject assumption II [4, 13]. For instance, Jaynes put forward the following derivation of the second law [3]: Start with an initial observation of an observable, \( M_0 = m_0 \). Confine ourselves to distributions \( \rho \) which have \( \langle M \rangle_\rho = m_0 \); call the set of such distributions \( C_0 \). Let the member of \( C_0 \) with the highest entropy be \( J_0 \); we select this as our initial distribution. Now let it evolve forward in time, giving \( T J_0 \); by assumption II \( H[J_0] = H[T J_0] \). The time evolution leads to a certain value for the observable, \( m_1 = \langle M \rangle_{T J_0} \). Now consider the class of distributions \( C_1 \) with \( \langle M \rangle_\rho = m_1 \); let the maximum entropy member of this class be \( J_1 \). Since \( T J_0 \in C_1 \), it follows that \( H[J_1] \geq H[T J_0] = H[J_0] \). Jaynes then identifies \( S_1 \) with \( H[J_1] \), i.e., he updates the distribution by re-applying the maximum entropy principle, using only the current observation, rather than by applying Bayes’s rule.

There are good reasons to doubt the wisdom of using probability as a measure of degree of belief [17]. But if you are going to do that, then the Bayesian way is the right way to do so, and you need to use conditioning. Failure to do so is incoherent, as the well-known “Dutch Book” arguments show. (17) gives a clear introduction; see [3] for details.) In particular, in the formally very similar problem of nonlinear filtering [17], application of Bayes’s rule is demonstrably optimal, and forgetting all earlier observations is not, regardless of whether one interprets probability subjectively.\(^3\)

\(^3\) The doubts raised by [18] about inter-temporal updating are not relevant. There’s no time lapse between \( TF_0 \) and \( F_1 \), just the addition of the information that \( M_1 = m_1 \).

Even if Bayesian statistical mechanics are free to not use conditioning, they still get a backwards arrows of time. A consistent use of the principle of maximum entropy, given the two observations \( M_0 = m_0 \) and \( M_1 = m_1 \), would go as follows. First, restrict ourselves to distributions \( \rho \) which satisfy both the constraints \( \langle M \rangle_\rho = m_0 \) and \( \langle M \rangle_{T \rho} = m_1 \). It is awkward to have one constraint on \( \rho \) and another on \( T \rho \); using the Koopman operator, we can turn the latter into a constraint on \( \rho \) as well, \( \langle U M \rangle_\rho = m_1 \). Let us write \( C_0 \) for the class of distributions satisfying these two constraints. Those satisfying the first constraint are the class we called \( C_0 \) above, and those satisfying the second constraint form a subclass of the set we called \( C_1 \) above. Hence \( C_{01} \subseteq C_0 \cap C_1 \). Then the maximum entropy principle tells us to pick the distribution \( J_{01} \) given by

\[
J_{01} = \arg \max_{\rho \in C_{01}} H[\rho] \tag{21}
\]

Since \( C_{01} \subseteq C_0 \) and \( C_{01} \subseteq C_1 \), it is clear that \( H[J_{01}] \leq \min H[J_0], H[J_1] \). Thus, updating our distribution by maximizing entropy, rather than conditioning, still reverses the arrow of time: by assumption III \( S_1 = H[T J_{01}] \), and by assumption II \( H[T J_{01}] = H[J_0] \leq H[J_0] = S_0 \).

To avoid getting the direction of the arrow of time backwards, the Bayesian or Jaynesian statistical mechanic must ignore the known prior history, a procedure quite without statistical justification. By use of the operator \( U \), constraints on a single observable over multiple times can be converted into constraints on multiple observables at a single time, which we are normally told must all be incorporated into the distribution \( F \). There does not seem to be any reason why it should be legitimate to take \( M \) as a constraint in the maximum entropy procedure, but not \( U M \). Worse yet, under some circumstances subjectivists (e.g., Jaynes, in his discussion of spin-echo experiments [2, 3]) have been explicit about needing to incorporate historical information in order to avoid unphysical predictions.

Whether we update via conditioning, or by applying the maximum entropy principle, we get unphysical results for the entropy, and can avoid them only by inconsistency about whether historical data counts, or, equivalently, whether all observables must inform the postulated distribution. One might argue that, for most systems of interest, the distribution obtained from applying the maximum entropy principle only to ordinary observables at the current time leads to nearly the same predictions as the coherent procedures, but the former is much easier to calculate than the latter, particularly if the dynamics are very irregular. In such a case, the complexity of computing the \( n \)^{th} iterate of the evolution operator, \( T^n \), may grow rapidly with \( n \), so that a computationally-limited agent, acting under time pressure, might prefer an approximation which neglects historical data to an exact but intractable update. The validity of such an approximation would depend on the ergodic properties of
the dynamics (e.g., mixing), and it is precisely to avoid such dependence that the Bayesian approach was introduced. Worse, it would lead to a novel kind of Maxwell’s demon, a purely passive observer who can make the entropy decrease during a time interval which depends on the observer’s processing speed and the time-complexity of computing $T_n$. In any event, none of this would explain why the thermodynamic entropy should match the entropy of this approximate distribution.

C. Assumption III Thermodynamic Entropy Is Subjective Uncertainty

Assumption III is that thermodynamic entropy $S$ is the information-theoretic uncertainty $H[F]$. Denying this seems to me a completely satisfactory option. Macroscopically, entropy is defined by its relations to the observables of heat and temperature. Microscopically, assuming the usual representation of phase space, entropy is the logarithm of the volume in phase space compatible with the current macroscopic state $\text{[19, 20, 21]}$; more generally, it is the logarithm of the measure of that region $\text{[22, 23]}$.

Rejection of assumption III is perfectly compatible with accepting a Bayesian, subjectivist interpretation of probability.

III. CONCLUSION

A backwards arrow of time follows directly from the combination of assumptions I, II and III, at least one of which must therefore be rejected. Rejecting assumption I, invertible microphysical dynamics, entails considerable modification of basic physics. Rejecting assumption II, updating subjective probabilities via Bayes’s rule, is actually insufficient; one must also reject the principle of maximum entropy, or at the very least apply it in an incoherent way, sometimes taking into account all observational constraints, sometimes not. Rejecting assumption III, the identification of thermodynamic entropy with the Shannon information $H[F]$, seems to lead to the least trouble. I do not pretend that only one choice among these alternatives is defensible, but some choice is necessary.

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