Is the Information Entropy the Same as the Statistical Mechanical Entropy?

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(Dated: 17 September, 2012. arXiv:cond-mat)

It is shown that the standard expression for the information entropy, originally due to Shannon, is only valid for a particular set of states. For the general case of statistical mechanics, one needs to include an additional term in the expression for the entropy as a function of the probability. A simple derivation of the general formula is given.

1. Introduction

For a system that can exist in states \( i = 1, 2, \ldots, n \) with probability distribution \( p \equiv \{p_1, p_2, \ldots, p_n\} \) that is normalised, \( \sum_{i=1}^{n} p_i = 1 \), the information entropy is

\[
S[p] = -k_B \sum_{i=1}^{n} p_i \ln p_i. \tag{1}
\]

Boltzmann’s constant, \( k_B \), is often suppressed in information applications, and the base of the logarithm is often taken to be 2. The information entropy is a measure of the disorder or lack of predictability of the system.

This formula for the entropy was originally introduced by Shannon as a way of quantifying the information content of messages.\(^1\) (Actually the same formula was also given by Gibbs\(^2\) who called it the average of the index of probability. It also coincides with Boltzmann’s H-function.) The formula remains standard in information theory. It is also widely used to calculate the entropy in statistical mechanics. Shannon’s implicit assumption—that this information entropy is the same as the entropy that is used in thermodynamics and in statistical mechanics—has generally been accepted unquestioned, and the formula has been used without modification in the physical sciences. Jaynes based his maximum entropy formulation of statistical mechanics (wherein the appropriate probability distribution is obtained by maximising the information entropy subject to certain constraints) on Eq. (1)\(^2\) and went on to use it as the basis of a novel interpretation of logic and probability that has widespread ramifications.\(^5\) It is also worth mentioning that statistical mechanical expansions have been used to develop efficient methods for evaluating the information entropy, Eq. (1)\(^2\)\(^2\).

This note examines in detail Shannon’s derivation of Eq. (1)\(^2\)\(^2\) which remains the standard text-book derivation.\(^9,10\) In Sec. 2 it is shown that the formula neglects the internal entropy of the states, due to a certain confusion between the total entropy and the entropy as a functional of the macrostate probability. In Sec. 3 a simple derivation of the full result is reproduced\(^11,13\) and in Sec. 4 it is discussed why this additional term is essential to obtain the correct physical results and agreement with the thermodynamic and the statistical mechanical entropy.

2. Derivation of the Information Entropy

Following Shannon’s original derivation (see Appendix 2 of Ref. 1, or Refs 6,10), and changing only the notation and adding a few clarifying remarks, the derivation of the formula for the information entropy is based on several self-evident axioms: that it is a continuous function of the \( p_i \), that it increases with the number of states in the uniform case, and that different ways of grouping the states must give the same value.

To understand this last axiom define a microstate as a complete set of distinct, disjoint, and indivisible states, and a macrostate as a set of microstates. Let \( i \) label the microstates used above, with probabilities \( p_i \), and let \( I \) label the macrostates. The macrostate \( I \) contains \( n_I = \sum_{i \in I} p_i \) microstates, and its probability is \( q_I = \sum_{i \in I} p_i \). The conditional probability of a microstate in a given macrostate is \( p_{i|I} = p_i/q_I \), \( i \in I \), which can be written as the \( n_I \)-component vector \( \{p_{i|I}\} \). In view of this definition, the total entropy can be written as the uncertainty due to the macrostate probability distribution, plus the additional uncertainty due to locating the microstate within each macrostate,

\[
S[p] = S[q] + \sum_I q_I S[\{p_{i|I}\}]. \tag{2}
\]

The last axiom says that no matter how the microstates are grouped into macrostates, the total entropy must remain unchanged.

This equation is written in the standard form (see, for example, Eq. (11.8) of Ref. 6, or the penultimate equation of Appendix 2 of Ref. 1), but there is a subtle ambiguity with it that ultimately causes the problem with the information entropy. On the one hand, the notation implies that the entropy expressed as a functional of the microstate probability on the left hand side, \( S[p] \), is the same function of its argument as the entropy expressed as a functional of the macrostate probability on the right hand side, \( S[q] \). On the other hand, the left hand side of the equation implies that the microstate form \( S[p] \) is the total entropy of the system, whereas the right hand side implies that the macrostate form \( S[q] \) is only part of the total entropy of the system. The expression for the information entropy, Eq. (1), results from overlooking this distinction, as is discussed below.

Following Shannon’s Appendix 2\(^1\) or Jaynes’ Eq. (11.10)\(^2\) assume that the microstates are equally
likely, $p^u = 1/n$, so that the left hand side of Eq. (2) is

$$S[p^u] = \sigma(n).$$

(3)

Further assume that the macrostates are all the same size, $n_I = m$, so that $q_I = m/n$ and $\sigma_I = 1/m$. Hence $S[q^u] = \sigma(n/m)$ and $S[p_i/q_I] = \sigma(m)$. With these two assumptions Eq. (2) becomes

$$\sigma(n) = \sigma(n/m) + \sum_I q_I \sigma(m)$$

$$= \sigma(n/m) + \sigma(m).$$

(4)

This has evident solution

$$\sigma(n) = k_B \ln n.$$  

(5)

Apart from the choice of Boltzmann’s constant and the logarithmic base, this solution is unique. This result may be seen to be consistent with Boltzmann’s original definition of the entropy, namely that the entropy of a state is the logarithm of the number of molecular configurations in the state, assuming that the configurations are all equally likely.

Now in order to deduce the form of the information entropy as a functional of the probability distribution, continue to take the microstates to be equally probable, $p^u = 1/n$, but now take the the macrostate distribution to be non-uniform, $q_I \neq q_J$. This is achieved by grouping different numbers of microstates $n_I$ into each macrostate $I$. In this case rearranging Eq. (2) yields

$$S[q] = S[q^u] - \sum_I q_I S[p_i/q_I]$$

$$= \sigma(n) - \sum_I q_I \sigma(n_I)$$

$$= -k_B \sum_I q_I \ln q_I,$$  

(6)

since $q_I = n_I/n$. With the apparently trivial replacement $I \rightarrow i$, this is the standard expression for the information entropy, and so this appears to be a straightforward and unambiguous derivation of Eq. (1).

However, as noted above, there is a conceptual problem with Eq. (2), namely that the notation implies that the microstate form $S[p]$ and the macrostate form $S[q]$ are the same functions of their arguments, whereas the content of the equation implies that $S[p]$ is the total entropy whereas $S[q]$ is only part of the total entropy. The only way to resolve this discrepancy is to rewrite Eq. (2) in terms of the macrostate probability with the total entropy explicit,

$$S_{\text{total}} = S[q] + \sum_I q_I S[p_i/q_I].$$

(7)

The total entropy has to be independent of how the microstates are grouped into macrostates, (Axiom 4). Hence this result can also be used when the macrostates are taken to be microstates themselves (i.e. one microstate in each macrostate), in which case this becomes

$$S_{\text{total}} = S[p] + \sum_i q_i S[p_i/q_i] = S[p] + \sum_i p_i \sigma(1).$$

(8)

The simplest assumption is that there is no uncertainty for a system consisting of a single microstate, $\sigma(1) = 0$. (This assumption will be revisited in the next section.) With these two equations, most of the preceding analysis holds. Assuming a uniform distribution of both microstates and macrostates one again finds that $S_{\text{total}} = \sigma(n) = k_B \ln n$. Assuming non-uniform macrostates, $q_I \neq q_J$, and uniform microstates, $p^u = 1/n$ does not change the total entropy, $S_{\text{total}} = k_B \ln n$. In this case Eq. (7) may be rearranged as

$$S[q] = k_B \ln n - \sum_I q_I \sigma(n_I) = -k_B \sum_I q_I \ln q_I.$$

(9)

This has the appearance of the standard information entropy result, but now Eq. (7) shows explicitly that this is only part of the entropy of the system. Inserting this into Eq. (7) gives the total entropy as

$$S_{\text{total}} = -k_B \sum_I q_I \ln q_I + \sum_I q_I S_I,$$

(10)

where in this case the internal entropy of the macrostate for equally likely microstates is $S^u_I = S[p_i/q_I] = \sigma(n_I)$. (This explicit result for the internal entropy of the macrostate does not hold if the microstates are non-uniformly distributed, but Eq. (10) does hold in this general case, as is shown in the next section.)

This formula remains predicated on the assumption that the underlying microstates are uniformly distributed. A derivation will be given in the following section without this restriction. Before then however two comments can be made. First, if the microstates are in reality uniformly distributed, $p^u = 1/n$, then it turns out that the internal entropy of a macrostate can indeed be taken to be zero, $S^u_i = 0$, and this result for the total entropy expressed in terms of microstates reduces to the information entropy form, Eq. (1). In this case the result is trivial

$$S_{\text{total}} = -k_B \sum_i p_i \ln p_i = k_B \ln n.$$

(11)

Because this result is trivial (and in essence just a statement of Boltzmann’s original definition of the statistical mechanical entropy) there really is no point in formulating the total entropy in the information entropy form for uniformly distributed microstates.

Second, although both Eq. (9) and Eq. (10) are true for non-uniformly distributed macrostates, the derivation depends upon the microstates being uniformly distributed. Additional assumptions or a different derivation is required when the microstates are not uniformly distributed. Similarly, there is nothing in the derivation that says that either of these two equations can
be applied to non-uniformly distributed microstates (i.e. \( I \mapsto i \)), which Shannon and Jaynes \( ^{14,15} \) both assume in their derivation of Eq. (11).

3. Derivation for Non-Uniform Microstates

A simpler and more general (in the sense that it applies for non-uniformly distributed microstates) derivation of the entropy as a functional of the probability distribution has been given by the author. \( ^{14,15} \) Suppose that the microstate \( i \) has weight \( w_i \). These weights arise from the molecular details of the problem and they need not be specified explicitly beyond the fact that they are non-negative and linearly additive, which are required for the system to satisfy the laws of probability.

Because the states are distinct, disjoint, and complete, and because the weights are linearly additive, the weight of a macrostate is \( W_I = \sum_{i \in I} w_i \), and the total weight is

\[
W = \sum_i w_i = \sum_I W_I. \tag{12}
\]

The probability of a state is proportional to its weight,

\[
p_i = \frac{w_i}{W}, \quad \text{and} \quad q_I = \frac{W_I}{W}. \tag{13}
\]

These are obviously normalised. The total weight is called the partition function in statistical mechanics.

Weight is the obvious generalisation of number in the case that the states are not equally likely. Hence the entropy of a state is defined to be Boltzmann’s constant times the logarithm of the weight of the state. The microstate, macrostate, and total entropy are

\[
S_i \equiv k_B \ln w_i, \quad S_I \equiv k_B \ln W_I, \quad \text{and} \quad S_{\text{total}} \equiv k_B \ln W. \tag{14}
\]

respectively. It turns out that the entropy defined like this has all the properties that one would desire of the entropy in physical systems. The logarithm makes entropy an extensive variable, like energy, number, and volume, and this is what makes it so convenient for thermodynamics and statistical mechanics.

In view of the relationship between entropy and weight, the probability of a state is proportional to the exponential of the entropy divided by Boltzmann’s constant,

\[
p_i = \frac{e^{S_i/k_B}}{W}, \quad \text{and} \quad q_I = \frac{e^{S_I/k_B}}{W}. \tag{15}
\]

This generic relationship between entropy and probability is well known in statistical mechanics.

Now to the major result, namely the information entropy for the case of non-uniform probability distributions. In view of the normalisation of the probability distributions it is straightforward to verify that

\[
S_{\text{total}} = k_B \ln W
\]

\[
= k_B \sum_i p_i \ln W
\]

\[
= k_B \sum_i p_i \left[ \ln \frac{W}{w_i} + \ln w_i \right]
\]

\[
= -k_B \sum_i p_i \ln p_i + \sum_i p_i S_i. \tag{16}
\]

In the above formulation there was no fundamental distinction between macrostates and microstates, and so the total entropy can equivalently be written as a functional of the macrostate probability,

\[
S_{\text{total}} = -k_B \sum_I q_I \ln q_I + \sum_I q_I S_I. \tag{17}
\]

These are in the form of Eq. (11) (for both microstates and macrostates) but not in the form of the information entropy expression, Eq. (1).

4. Discussion

This obvious contradiction between the information entropy result Eq. (1) and the statistical mechanical entropy result, Eq. (16), or Eq. (17), raises the question: when is it valid to neglect the internal entropy of the states?

For the case that the microstates are equally likely, one can indeed set their weight to unity, \( w_i = 1 \), and their entropy to zero, \( S_i = 0 \). But in this case Eq. (1) reduces to the trivial result, \( S_{\text{total}} = k_B \ln n \), and there is no circumstance when the formula in terms of the probability distribution is required.

In the case that the microstates are not equally likely, one cannot neglect their internal entropy without explicit justification. In statistical mechanics the generic cases where the microstates are not equally likely usually involve hidden variables that are projected out of the problem. One example is where one describes the microstates of the system in terms of molecular coordinates (e.g. the position and momenta of the center of mass of the molecules). This neglect finer levels of description, (e.g. the rotational coordinates, the bending and stretching of, and the rotation about intramolecular bonds, the electron configuration, etc.). Depending upon the specific system, there may be good reason for neglecting such finer levels of description, and there may also be good reason for neglecting the internal entropy due to them (e.g. the internal configurations and their weight might be the same for all the microstates, and so the internal entropy might be constant).

The second example of the microstates having an internal entropy is where the total system consists of a sub-system and a reservoir, and the coordinates of the sub-system form the microstates. For example, the canonical equilibrium system is that of a sub-system in contact with a thermal reservoir of temperature \( T \). Here the microstates are the points in the phase space of the
Sated with each phase space point of the sub-system is points of the reservoir, and the internal entropy associated with each phase space point of the sub-system is $S(\Gamma) = -\mathcal{H}(\Gamma)/T$, where $\mathcal{H}$ is the Hamiltonian or total energy of the sub-system. This may be recognised as the change in entropy of the reservoir. Neglecting this microstate entropy by using the information theory expression, Eq. (1), would give the wrong total entropy for the canonical equilibrium system. With the Maxwell-Boltzmann distribution, $\varphi(\Gamma) = Z^{-1} \exp -\mathcal{H}(\Gamma)/k_B T$, the information entropy form gives the total entropy as

$$
\tilde{S}_{\text{total}} = -k_B \int d\Gamma \varphi(\Gamma) \ln \varphi(\Gamma) = k_B \ln Z + \frac{1}{T} \langle \mathcal{H}(\Gamma) \rangle,
$$

(18)

whereas the full expression gives

$$
S_{\text{total}} = \int d\Gamma \varphi(\Gamma) [-k_B \ln \varphi(\Gamma) + S(\Gamma)] = k_B \ln Z.
$$

(19)

Clearly, only the full expression agrees with the well-known result that the logarithm of the partition function gives the total entropy of the system. The information entropy expression gives the entropy of the sub-system alone, neglecting the reservoir entropy. Obviously, in seeking, for example, to optimise a system, one should maximise the total entropy, not just part of it.

From this example, one can see explicitly why the information entropy expression, Eq. (1), is inappropriate for statistical mechanics. The question remains: in what sense is it appropriate for information theory?

The information entropy singles out a particular representation as the preferred representation, namely the one in which $\sum_i p_i S_i = 0$. Since only differences in entropy are significant, it is always possible to add a constant to the entropy,

$$
\tilde{S}_i = S_i + c, \quad \tilde{S}_f = S_f + c, \quad \text{and} \quad \tilde{S}_{\text{total}} = S_{\text{total}} + c. \quad (20)
$$

Choosing $c = -\sum_i p_i S_i$ (either explicitly or implicitly), one sees that

$$
\tilde{S}_{\text{total}} = -k_B \sum_i p_i \ln p_i = -k_B \sum_i q_i \ln q_i + \sum_i q_i \tilde{S}_i.
$$

(21)

The first equality is in the form of the information entropy, but the second equality shows that any shift to another set of states requires the full expression for the total entropy.

In communications and informatic problems, one generally does not have an underlying molecular description of the message, signal, image, etc., and so one cannot give the actual value of the weight or the entropy of a state. However, one can measure the probability of a state with relative ease. The apparent advantage of Eq. (1) and of the first equality here is that it depends only on the probability distribution, not explicitly upon the entropy of the states. Further, it is often the case that the microstates are chosen based on the individual characters in a message (or the pixels in an image), and these are indivisible and arguably have no internal rearrangement that can contribute to the information content of the message. In this sense one can make a strong argument for applying Eq. (1) in informatic applications provided that one explicitly restricts its use to such microstates. One should not use that particular equation in statistical mechanics because it risks confusion between microstates and macrostates, and also because it is not valid for the microstates that typically appear in statistical mechanics.

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