Maximum Entropy, Time Series and Statistical Inference

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ABSTRACT: A brief discussion is given of the traditional version of the Maximum Entropy Method, including a review of some of the criticism that has been made in regard to its use in statistical inference. Motivated by these questions, a modified version of the method is then proposed and applied to an example in order to demonstrate its use with a given time series.
1. Historical Background

The concept of entropy has gone through several distinct stages since its inception in the 19th century. Originally formulated as a thermodynamic potential, Boltzmann reexpressed it as a measure of disorder. The connection between thermodynamics and disorder, or randomness, is given by Boltzmann’s ansatz \( S = \log(W) \) where \( W \) is the count of accessible configurations

\[
W = \frac{N!}{\prod_i n_i!}
\]

and which leads to the expression

\[
S = - \sum_i p_i \log(p_i)
\]

where \( p_i \) is the Boltzmann factor for the \( i^{th} \) energy state. In the 20th century, through the work of Shannon [1] and Wiener [2] a second application was developed where this same expression came to be used as a measure of the amount of information contained in a string of characters each of frequency or probability \( p_i \).

The conceptual association of disorder and information as opposites was a natural one to make, but there is considerable disagreement as to how these two ideas, thermodynamic entropy and information, are related. Beginning with Szilard [3], a direct connection between entropy decrease and information gain was made suggesting that the two differ only by a sign. Recently Zurek [4] has proposed a more complicated relation suggesting that gain in information is not entirely reflected in the loss in entropy. We will come back to the question information and entropy later.

2a. Maximum Entropy and Inference

Dating from his paper of 1957 [5], ET Jaynes presented a third use for the expression for entropy, employing it as a tool for statistical inference. Consider the problem of constructing the probability distribution of a system when we have obtained data/measurements in the form of a set of \( M \) numerical values \( \{x_i\} \). With the above definition of entropy and a constraint on the extremum of the form

\[
m_1 = \sum_i p_i x_i
\]

(where \( m_1 \) the first moment) then the full entropy might be written

\[
S = - \sum_i p_i \log(p_i) + \lambda \sum_i p_i x_i
\]

with \( \lambda \) the Lagrange multiplier, and calculating \( \delta S = 0 \) we obtain

\[
p_i = \frac{e^{\lambda x_i}}{Z}, Z = \sum_i e^{\lambda x_i}
\]

The undetermined multiplier is obtained from

\[
m_1 = \frac{\partial \log(Z)}{\partial \lambda}.
\]
This set of formulae is directly analogous to the steps taken in statistical mechanics that relate temperature to the multiplier in equilibrium physics. The algorithm for constructing the distribution using data is apparently straightforward, but as it turns out, there have been a number of critics over the years who have questioned Jaynes’ formalism.

2b. Criticism of the Maximum Entropy Formulation

In the traditional ME formulation a strict analogy is made between the microscopic presentation of statistical mechanics, of which the Boltzmann factor is the principle result, and statistical inference. As Jaynes would have it, this is exactly what one must do for statistical inference; given a time series whose average is known, one must maximize

\[ S = \sum_i p_i \log(p_i) + \lambda \sum_i p_i x_i \]

where the time series of values \( x_j \) has been replaced by

\[ \sum_j x_j \rightarrow \sum_i n_i x_i. \] (2)

In this expression, the \( M \) observed values of \( x_j \) are tabulated and then expressed as a sum of \( n_1 \) occurances of \( x_1 \), \( n_2 \) occurances of \( x_2 \), \( n_3 \) occurances of \( x_3 \),.... There are several things wrong with this:

1. It is necessary to make a replacement of frequencies with probabilities as in eq 2, which contradicts the position that probabilities need not always be associated with frequencies.
2. In the variation of \( S \) in statistical mechanics, the constraint is made up of variables \( n_i \) over which the variation is taken; in ME, the constraint is made up of data values, which are not free to be varied.
3. There have been several additional criticisms of the ME method beginning with Friedman and Shimony [4,5,6,7]. Good reviews of these questions can be found in Uffink [7]. In particular, FS find an inconsistency in ME with respect to its Bayesian properties. It will be shown below that the ME formalism will not always reproduce the mean value of the data correctly, and will generally produce a different standard deviation.

2c. Modified Maximum Entropy

If we confine the theory to time series data only, a corrected version of ME is easily obtained. Consider the following prescription for statistical inference. Given a time series \( x_j \) of \( M \) values we consider the total number of configurations as

\[ W = \frac{N!}{\prod_i n_i!} \]
and then weight this product by an extra factor

\[ W \rightarrow \frac{N!}{\prod n_i!} Q \]

where

\[ Q = p^{m_1}(x_1)p^{m_2}(x_2)\ldots p^{m_N}(x_N) \]

which is the probability of a particular string of observations \( \{x_j\} \). That is, \( m_i \) is the number of times \( x_i \) has appeared in the time series. Then the maximization leads to

\[ \delta S = 0 = \sum_i \delta S_i \]

where each contribution to the sum is of the form

\[ S_i = -p_i \log(p_i) + m_i \log(p_i) \]

and where the first term (the entropy part) arises from the count of configurations \( W \), and the last term (the informational part) from the weight \( Q \). The minimization procedure results in an expression for the probability (disregarding normalization)

\[ p_i = \exp\left(\frac{m_i}{p_i}\right) \]  \hspace{1cm} (3)

which may be solved iteratively for \( p_i \), yielding

\[ p(n) = \frac{n}{Z(n)} \]

where

\[ Z(n) = \log(n) - \log(\log(n)) + O\left[\frac{\log(\log(n))}{\log(n)}\right] \]

Generally, in the case that successive elements of the time series cannot be treated as independent, we must use the above equation to solve for \( p(n_1, n_2) \), \( p(n_1, n_2, n_3) \), etc., depending on the nature of the correlations in the time series. The evaluation of \( W \) in this case is somewhat more involved, but that of \( Q \) remains the same.

3. Example Application
3a. Traditional ME

One of the obvious failings of ME is that it does not reflect the different contribution made by a short time series versus that of a long one. In particular, if the data consisted of a single coin toss, there does not appear to be a formal solution of the evaluation of the Lagrange multiplier, i.e. equation 1. The following is an example of this difficulty (see also Uffink 1996).

Suppose we have a three sided coin \( x_i = 1, 2, 3 \) and toss it several times with the result \( m_1 \). This is the first few elements in a time series and ought to provide a first estimate in the probabilities of the three sides. According to the above algorithm, the Lagrange multiplier for this problem is

\[ m_1 = \frac{x_1q + x_2q^2 + x_3q^3}{Z} \]
where \( q = e^{-\lambda} \). The prescription is to solve for \( \lambda \), that is

\[
(m_1 - x_1)q + (m_1 - x_2)q^2 + (m_1 - x_3)q^3 = 0
\]

(4)

A plot of the largest real positive root is given in Figure 1. If the time series contains only a few elements, it is possible that the average turns out to be \( m_1 = 1 \) or \( m_1 = 3 \) yet according to the plot this requires \( q = 0 \) or \( q = \infty \), i.e. no disorder regardless of the data.

This difficulty extends to the moments in general. For example, for a two level system with "energies" \( \epsilon_1, \epsilon_2 \), in Jaynes’ formulation, moments are determined from data

\[
m_l = \sum_j x_j^l
\]

and these in turn are related to the Lagrange multipliers by

\[
m_l = \frac{1}{Z} \left[ \epsilon_1^l e^{\phi_1} + \epsilon_2^l e^{\phi_2} \right]
\]

with

\[
Z = e^{\phi_1} + e^{\phi_2}
\]

where the multipliers are given by

\[
\phi_i = \lambda_1 \epsilon_i + \lambda_2 \epsilon_i^2 + \lambda_3 \epsilon_i^3 + \ldots
\]

For the two-level system, this works out to be

\[
\frac{(m_l - \epsilon_1^l)}{(m_l - \epsilon_2^l)} = e^{\phi_2 - \phi_1}
\]

for all \( l \), which is overdetermined in general and so has no solution.
3b. Modified ME

In contrast the modified method yields probability values for any length of time series, and in the limit of a large string, gives the same value as would be obtained from a direct frequency tabulation. As a demonstration of how this operates, consider the toss of a two-sided coin, using a possibly biased coin. After \( N = n_h + n_t \) tosses the probability for each side is given by

\[
P_h = \frac{p(n_h)}{p(n_h) + p(n_t)} \quad \text{and} \quad P_t = \frac{p(n_t)}{p(n_h) + p(n_t)},
\]

where \( p(n_h) \) is the solution to equation 3 above.

Normalization of the probabilities is given by

\[
Z = p_h(n_h) + p_t(n_t)
\]

The case similar to the one described above by Uffink is where a single toss results in a head which is obtained from

\[
Z = p_h(1) + p_t(0)
\]

In Figure 2 we plot the probability of heads and tails respectively, in a simulation where the coin is biased such that in the infinite limit we should have \( p_h = .7 \) and \( p_t = .3 \). As can be seen the initial values are rough, while in the limit of large data the values go over into the frequency values.

Returning now to the problem discussed above, consider a 2-sided coin that can only land heads up, such that successive throws yield an increasingly long string of heads. Regardless of the string length, the traditional ME can only give the solution \( (p_h, p_t) = (1, 0) \), as shown in Section 3a, while the modified version gives \( p_t = 1 - p_h \) and

\[
p_h = \frac{p(n)}{1 + p(n)}
\]

after the \( n^{th} \) throw. This is plotted in Figure 3 and provides a more realistic description of how an experimenter might gradually, but inevitably, come to the conclusion that the toss is not random.
4. Discussion

In summary we have proposed that the traditional method of applying the Maximum Entropy method, which involves maximization of

$$S = -\sum_i p_i \log(p_i) + \lambda \sum_i p_i x_i$$

must be modified to

$$S = -\sum_i p_i \log(p_i) + \sum m_i \log(p_i)$$

when dealing with time series. This allows the elements of a time series, no matter how few in number, to be included and hence influence the resulting distribution. This method has several advantages, most notably that the elements of the time series can be put into the computation without difficulty and without complication whether the series is short or long. Also, as the series becomes very long, the probability values become equal to those found from direct frequency tabulation. One undeniable disadvantage is that the resulting distribution is not usually a smooth function of the data. That is, for a short series, a small number of new data points may make a considerable change in the numerical values of the $p_i$; this is in contrast with the traditional ME approach, but perhaps is a more realistic property of statistical inference.

The modified expression is made up of an entropy component and an informational one. For short time series with little or no data, the entropy contribution dominates, starting off with the equal probability distribution when no data at all is at hand. Then, as data is accumulated (the longer time series), the informational part dominates, and it is to be expected that the manner of cross-over from one to the other should depend on the nature of the data. The interpretation of this is easily seen by considering the example of the completely biased coin where $p_h = 1$. The information obtained from a single toss is given by $p_h \log(p_h) + p_t \log(p_t) = 0$; this makes sense as the outcome is already known; however, we might ask how much information had been acquired in determining the distribution originally? The results obtained here suggest that the additional term in the expression for
entropy provides a means of fixing a value to the information contained in the statement of the distribution. These ideas are somewhat in line with earlier studies (Zurek [4], Lin [10]), though the context of this added term is different from these papers. In order to find how much information is already contained in the knowledge of the distribution, we must consider the manner in which the distribution was obtained. Initially we might start with $p_h = p_t = \frac{1}{2}$, and begin tossing, keeping record of the results. Each toss modifies $p_h$ and $p_t$ according to the function $p(n)$ given in equation 3. As the number of tosses grows indefinitely, the amount of information contained in the data is given by the limiting value shown above, $-n \log(p)$, which for the completely biased coin leads to $\log(n)$ for large $n$. 
Acknowledgment: I want to thank A. Shimony for making comments on an earlier version of this paper, and I also want to thank L. Bruch for his continued assistance and many offerings of good advice.

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