Maximum Entropy, Fluctuations and Priors*

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Abstract

The method of maximum entropy (ME) is extended to address the following problem: Once one accepts that the ME distribution is to be preferred over all others, the question is to what extent are distributions with lower entropy supposed to be ruled out. Two applications are given. The first is to the theory of thermodynamic fluctuations. The formulation is exact, covariant under changes of coordinates, and allows fluctuations of both the extensive and the conjugate intensive variables. The second application is to the construction of an objective prior for Bayesian inference. The prior obtained by following the ME method to its inevitable conclusion turns out to be a special case ($\alpha = 1$) of what are currently known under the name of entropic priors.

1 Introduction

The goal of inductive inference is to update a prior probability distribution to a posterior distribution when new information becomes available. The problem is to process this information in a systematic and objective way. When the information is in the form of constraints on the family of conceivable posterior distributions, there is one inference procedure that is singled out by requirements of universality, objectivity, and consistency: it is the method of maximum entropy (ME) [1]. The standard justification relies on interpreting entropy, through the Shannon axioms, as a measure of the amount of uncertainty in a probability distribution [2], but this justification is not entirely unobjectionable. A relatively minor problem is that the Shannon axioms refer to discrete probability distributions rather than continuous ones. A more serious one is that it is not clear that they provide the only way to define the notion of uncertainty. This has motivated a number of attempts to justify the ME method directly, without invoking questionable measures of uncertainty [3][4]. They have established the value of the concept of entropy irrespective of any interpretation in terms of heat, or disorder, or uncertainty. In these approaches entropy is purely a tool

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for consistent reasoning; strictly, *entropy needs no interpretation*. A welcome by-product has been that the entropy thus defined turns out to be directly applicable to continuous distributions. In Sect. 2, as background for the subject of this paper, we present a brief outline of one such ‘no-interpretation’ approach. Except for one slight modification we follow Ref.[4] closely.

The main body of the paper addresses three problems. The unifying element is the particular form of the constraints; unlike most applications of the ME method the constraints are not in the form of known expectation values of certain variables.

The first problem we tackle provides an extension of the ME method itself. Once one accepts that the maximum entropy distribution is to be preferred over all others, the question is to what extent, how strongly, are distributions with lower entropy supposed to be ruled out. In statistical mechanics the answer to this question is well known. It was first obtained on the basis of combinatorial arguments in the pioneering work of Boltzmann, it is the foundation on which Einstein formulated his theory of fluctuations and Onsager erected his theory of irreversible processes. More recently it was explored by Jaynes [5]. Our goal is to show (Sect. 3) that the answer can be obtained entirely from within the ME framework, without appeals to combinatorics, to large systems, or other forms of intuitive and/or approximate arguments.

The second problem turns out to be a special case of the first: we are concerned with the theory of fluctuations. The starting point for the standard theory (see e.g. Ref.[6]) is Einstein’s inversion of Boltzmann’s formula $S = k \log W$ to obtain the probability of a fluctuation in the form $W \sim \exp S/k$. A careful justification, however, reveals a number of approximations which, for most purposes, are legitimate and work very well. Later developments including the method of cumulants, the renormalization group, and the connection to non-equilibrium thermodynamics succeeded in clarifying most of the remaining conceptual and calculational issues.

A re-examination of fluctuation theory from the point of view of ME is, however, valuable. Our general conclusion (Sect. 4) is that the ME point of view allows exact formulations; in fact, it is clear that deviations from the canonical predictions can be expected, although in general they will be negligible. Other advantages of the ME approach include the explicit covariance under changes of coordinates, the absence of restrictions to the vicinity of equilibrium or to large systems, and the conceptual ease with which one deals with fluctuations of both the extensive as well as their conjugate intensive variables. This last point is an important one: within the canonical distribution the extensive variables are random variables while the intensive ones are fixed parameters, they do not fluctuate. There are, however, several contexts in which it makes sense to talk about fluctuations of the conjugate variables. We discuss the standard scenario of an open system that can exchange say, energy, with its environment. An altogether different interpretation, which we will not discuss here, is to consider fluctuations in conjugate variables as uncertainties in the estimation of parameters [7].

The third, and last problem we address is that of obtaining an objective
prior for use in Bayes’ theorem. The goal is to obtain information about an unknown quantity \( \theta \) on the basis of the observed value of another quantity \( x \) and of a presumably known relation between \( x \) and \( \theta \). This is achieved through Bayes’ theorem, \( p(\theta|x) \propto \pi(\theta)p(x|\theta) \). The relation between \( x \) and \( \theta \) is supplied by a known model \( p(x|\theta) \); previous knowledge about \( \theta \) is codified into the prior probability \( \pi(\theta) \).

The selection of a definite prior is a famously controversial issue. It has generated an enormous literature \([11]\). The difficulty lies not so much in a lack of knowledge about \( \theta \), but rather in that this knowledge is sometimes vague: it is not clear how to codify it in an objective way. Faced with this difficulty one reasonable attitude is to admit subjectivity, and recognize that different individuals may legitimately translate the same vague information into different prior distributions.

An alternative attitude has been to seek some objectivity by demanding properties such as invariance under reparametrization or other symmetry transformations. Considerable effort has been spent searching for that special state of knowledge characterized by complete ignorance, and accordingly, there are a number of proposals based on the notion of missing information \([12]-[13]\). In the end, it may turn out that such a search is misguided; non-informative priors might not exist \([16]\).

A more positive, direct approach is to identify the information that we do in fact possess and then find an objective way to take it into account. Remarkably, it turns out that the very conditions that led us to contemplate using Bayes’ theorem constitute information that can be objectively translated into a prior using the ME method. The prior thus obtained (Sect. 5) turns out to be one particular member of the family of distributions known as “entropic priors.” The name and the first derivation of this family for the case of discrete distributions are due to Skilling \([13]\). The generalization to the continuous case and further elaborations by Rodríguez appear in Ref. \([14]\). The immediate motivation for the present work is found in Ref. \([15]\).

## 2 The logic behind the ME method

Let our beliefs about \( x \in X \) be codified in a probability distribution \( m(x) \). When new information becomes available we want to revise \( m(x) \) to a posterior distribution \( p(x) \). The ME method is designed to guide us in selecting \( p(x) \) when the new information is in the form of a specification of the set of acceptable posterior distributions. The \textit{information} is just a constraint on the region in the space of all distributions where the search will be carried out. (These constraints can, but need not, be linear.)

The selection is carried out by ranking the probability distributions according to increasing \textit{preference}. Two desirable features to be imposed on this ranking scheme are the following. The first is a transitivity requirement: if distribution \( p_1 \) is preferred over distribution \( p_2 \), and \( p_2 \) is preferred over \( p_3 \), then \( p_1 \) is preferred over \( p_3 \). Such transitive rankings can be implemented by assigning
a real number \( S[p] \) to each \( p(x) \), in such a way that if \( p_1 \) is preferred over \( p_2 \), then \( S[p_1] > S[p_2] \). The real number \( S[p] \) will be called the entropy of \( p(x) \). (Thus entropies are real numbers by design.) The selected \( p \) will be that which maximizes \( S[p] \). (Thus maximum entropy.)

The problem of finding the functional form of \( S[p] \) brings us to the second desirable feature to be imposed on the ranking scheme. We are looking for a general rule of inference; the ranking procedure, the rule \( S[p] \), must be of universal applicability: the same rule must apply to a variety of different cases. If we happen to know what the selected distribution should be in a certain special case, then this knowledge can be used to constrain the form of \( S[p] \). If enough special cases are known \( S[p] \) will be completely determined. These special cases – the so-called axioms – must, by their very nature, be self-evident.

Four axioms are listed below. They all reflect the conviction that changing one’s mind is a serious matter, that one should only update those aspects of one’s beliefs for which hard evidence has been supplied.

**Axiom 1: Subdomain independence.** If the space \( X \) is divided into non-overlapping subdomains \( D_i \), and information is given about \( p(x) \) for \( x \in D_1 \), the selection procedure should only revise the (relative) values of \( p(x) \) for \( x \in D_1 \). If the evidence makes no reference to \( x \not\in D_1 \) those values should be left unchanged. Non-overlapping subdomains are independent. The power of this axiom lies in that the choice of subdomains \( D_i \) is arbitrary, the consequence is that non-overlapping domains contribute additively to \( S[p] \).

**Axiom 2: Coordinate invariance.** The ranking should not depend on the particular system of coordinates being used. The coordinates used to label the points \( x \) do not carry any information. The consequence of this axiom is that the expression for \( S[p] \) will involve coordinate invariants such as \( dx \, p(x) \) and ratios such as \( p(x)/m(x) \), where the function \( m(x) \) is, at this point, any arbitrary measure.

**Axiom 3: Subsystem independence.** If a system is composed of two subsystems, \( x = (x_1, x_2) \in X = X_1 \times X_2 \), the selection procedure should introduce no correlations for which there was no evidence either in the measure or in the constraints. As a consequence of this axiom a logarithm appears in the expression for \( S[p] \).

**Axiom 4: Objectivity.** If there is no new information there is no reason to change one’s mind: when there are no constraints the selected posterior distribution should coincide with the prior distribution. The arbitrariness in \( m(x) \) is now removed: \( m(x) \) is the prior distribution.

The overall consequence of these axioms (for a proof see [4]) is that probability distributions should be ranked according to their entropy,

\[
S[p] = - \int dx \, p(x) \log \frac{p(x)}{m(x)}.
\] (1)

Choosing the prior \( m(x) \) can be tricky. When there is no information leading us to prefer one microstate of a physical system over another we might as well assign equal prior probability to each state. Thus it is reasonable to choose
the density of states as the prior distribution \( m(x) \); the invariant \( m(x)dx \) is the number of microstates in \( dx \). This is the basis for statistical mechanics.

Other examples of relevance to physics arise when there is no reason to prefer one region of the space \( X \) over another. Then we should assign the same prior probability to regions of the same “volume,” and we can choose \( \int_R dx m(x) \) to be the volume of a region \( R \) in the space \( X \). On the basis of this choice of prior one can derive a considerable amount of the formalism of quantum mechanics. This includes the “postulates” that quantum states form a Hilbert space, that probabilities are computed through the Born rule, and that time evolution is unitary [17].

Notice that through the measure \( m(x) \) Laplace’s principle of insufficient reason still plays a role, albeit in a somewhat modified form. Thus, subjectivity has not been eliminated. Just as with Bayes’ theorem, what is objective here is the manner in which information is processed, not the initial probability assignments.

3 Extending the ME method

Let \( X \) be the space of microstates \( x \) of a physical system \( (x \in X) \), and let \( m(x)dx \) be the number of microstates in the range \( dx \). (Although in this and in the next section we tend to drift into the language of statistical mechanics it will be clear that the central idea is easily exported to other contexts.) We assume that the expected values \( A^\alpha \) of some \( n_A \) variables \( a^\alpha(x) \) \((\alpha = 1, 2, \ldots, n_A)\) are known,

\[
\langle a^\alpha \rangle = \int dx p(x) a^\alpha(x) = A^\alpha. \tag{2}
\]

This limited information will certainly not be sufficient to answering all questions that one could conceivably ask about the system. Therefore, we make the further assumption that the set \( \{a^\alpha\} \) has not been randomly chosen, that it has been carefully selected because previous experience indicates the information in (2) is relevant for our purposes.

The probability distribution \( p_0(x) \) that best reflects the prior information contained in \( m(x) \) updated by the information \( A^\alpha \) is obtained by maximizing (1) subject to the constraints (2). The result is

\[
p_0(x) = \frac{1}{Z} m(x) e^{-\lambda_\alpha a^\alpha(x)}, \tag{3}
\]

where the partition function \( Z \) and the Lagrange multipliers \( \lambda_\alpha \) are given by

\[
Z(\lambda) = \int dx m(x) e^{-\lambda_\alpha a^\alpha(x)} \quad \text{and} \quad -\frac{\partial \log Z}{\partial \lambda_\alpha} = A^\alpha. \tag{4}
\]

The question we address concerns the extent to which the maximum entropy distribution \( p_0(x) \) should be preferred over other distributions with lower entropy. Consider a family of distributions \( p(x|\theta) \) which depends on a finite,
though arbitrarily large, number \( n_\theta \) of parameters \( \theta^i (i = 1, 2, \ldots, n_\theta) \) and which includes \( p_0(x) \) as one of its elements. We can choose the parameters \( \theta^i \) so that \( p(x|\theta = 0) = p_0(x) \).

The question about the extent that \( p(x|\theta = 0) \) is to be preferred over \( p(x|\theta \neq 0) \) can be phrased more suggestively as follows. To what extent do we believe that the correct selection should be \( \theta = 0 \) rather than \( \theta \neq 0 \)? Thus, our question has metamorphosed into an inquiry about a degree of belief: the probability of \( \theta, \pi(\theta) \). In fact, we should go further back. The original endeavor which led us to use the ME method in the first place was a question about the probability of \( x \), now we are actually asking about the probability of \( x \) and \( \theta \). We want not just \( p(x) \) but rather \( p(x, \theta) \); asking about the reliability of the answer \( p_0(x) \) has led us to expand the universe of discourse from \( X \) to \( X \times \Theta \) where \( \Theta \) is the space of parameters \( \theta \). It is remarkable that this is precisely the kind of question the ME method is designed to answer; the strategy is to determine the distribution \( p(x, \theta) \) by maximizing an entropy subject to whatever constraints are known to hold. To proceed we must address two questions: precisely what is the form of the entropy to be maximized, and second, what are the constraints on \( p(x, \theta) \).

No definition of entropy is complete until a measure over the space in question \( (X \times \Theta) \) is specified. Our starting point is that a priori there is no known connection between \( x \) and the arbitrary set of parameters \( \theta \). Since a measure must not by itself introduce correlations for which there is no evidence, the prior measure \( m(x, \theta) \) must be a product, \( m(x) \mu(\theta) \) of the known density of states \( m(x) \) and a still unknown measure \( \mu(\theta) \) over the space \( \Theta \). Thus, the entropy to be maximized is

\[
\sigma[p] = -\int dx \, d\theta \, p(x, \theta) \log \frac{p(x, \theta)}{m(x)\mu(\theta)}.
\]

(5)

Next we incorporate the crucial piece of information that gives meaning to the parameters \( \theta \) and establishes the relation between \( \theta \) and \( x \): the conditional probability \( p(x|\theta) \) is known. This has two consequences: First, the joint distribution \( p(x, \theta) \) is constrained to be of the form \( \pi(\theta)p(x|\theta) \). Notice that this constraint is not in the usual form of an expectation value. Second, the ambiguity in the choice of the measure \( \mu(\theta) \) in \( \Theta \) is resolved. The family of distributions \( p(x|\theta) \) induces a natural distance in the space \( \Theta \): \( d\ell^2 = g_{ij} d\theta^i d\theta^j \), where \( g_{ij} \) is the Fisher-Rao metric \( \left[ 3 \right] \)

\[
g_{ij} = \int dx p(x|\theta) \frac{\partial \log p(x|\theta)}{\partial \theta^i} \frac{\partial \log p(x|\theta)}{\partial \theta^j}.
\]

(6)

Accordingly we choose \( \mu(\theta) = g^{1/2}(\theta) \), where \( g(\theta) \) is the determinant of \( g_{ij} \). Having identified the measure and the constraints, we allow the ME method to take over.

The preferred distribution \( p(x, \theta) \) is chosen by varying \( \pi(\theta) \) to maximize

\[
\sigma[\pi] = -\int dx \, d\theta \, \pi(\theta)p(x|\theta) \log \frac{\pi(\theta)p(x|\theta)}{g^{1/2}(\theta)m(x)}.
\]

(7)
Assume $p(x|\theta)$ is normalized, $\int dx \, p(x|\theta) = 1$. Maximizing (7) with respect to variations $\delta \pi(\theta)$ such that $\int d\theta \, \pi(\theta) = 1$, yields

$$0 = \int d\theta \left(-\log \frac{\pi(\theta)}{g^{1/2}(\theta)} + S(\theta) + \log \zeta\right) \delta \pi(\theta),$$

where the required Lagrange multiplier has been written as $1 - \log \zeta$, and

$$S(\theta) = -\int dx \, p(x|\theta) \log \frac{p(x|\theta)}{m(x)}.$$  

Therefore the probability that the value of $\theta$ should lie within the small volume $g^{1/2}(\theta)d\theta$ is

$$\pi(\theta)d\theta = \frac{1}{\zeta} e^{S(\theta)} g^{1/2}(\theta)d\theta \quad \text{with} \quad \zeta = \int d\theta \, g^{1/2}(\theta) e^{S(\theta)}.$$  

Equation (10) is our main result. It tells us that, as expected, the preferred value of $\theta$ is that which maximizes the entropy $S(\theta)$ because this maximizes the scalar probability density exp $S(\theta)$. But it also tells us the degree to which values of $\theta$ away from the maximum are ruled out. For macroscopic systems the preference for the ME distribution can be overwhelming.

Note that the density exp $S(\theta)$ is a scalar function and the presence of the Jacobian factor $g^{1/2}(\theta)$ makes Eq.(10) manifestly invariant under changes of the coordinates $\theta^i$ in the space $\Theta$.

4 Fluctuations

Fluctuations of the variables $a^\alpha(x)$ or of any function $b(x)$ of the microstate $x$ are usually computed in terms of the various moments of the canonical ME distribution $p_0(x)$ given by Eqs.(3-4) (see, however, Ref.[10]). Within this context all expected values, such as the constraints $\langle a^\alpha \rangle = A^\alpha$ and the entropy $S(A)$ itself are fixed, they do not fluctuate. The corresponding conjugate variables, the Lagrange multipliers $\lambda^\alpha = \partial S/\partial A^\alpha$, do not fluctuate either.

The standard way to make sense of $\lambda$ fluctuations is to couple the system of interest to a second system, a bath, and allow exchanges of the quantities $a^\alpha$. All quantities referring to the bath will be denoted by primes: microstates $x'$, density of states $m'(x')$, variables $a'^\alpha(x')$, etc. Even though the overall expected value $\langle a^\alpha + a'^\alpha \rangle = A^\alpha_T$ of the combined system plus bath is fixed, the individual expected values $\langle a^\alpha \rangle = A^\alpha$ and $\langle a'^\alpha \rangle = A'^\alpha = A^\alpha_T - A^\alpha$ are allowed to fluctuate. The ME distribution $p_0(x, x')$ that best reflects the prior information contained in $m(x)$ and $m'(x')$ updated by information on the total $A^\alpha_T$ is

$$p_0(x, x') = \frac{1}{Z_0} m(x)m'(x') e^{-\lambda_0 (a^\alpha(x) + a'^\alpha(x'))}.$$  

But less than ME distributions are not totally ruled out; to explore the possibility that the quantity $A^\alpha_T$ is distributed between the two systems in a less than
optimal way we consider distributions $p(x,x',A)$ constrained to the form
\begin{equation}
  p(x,x',A) = \pi(A)p(x|A)p(x'|A_T - A),
\end{equation}
where
\begin{equation}
  p(x|A) = \frac{1}{Z(\lambda)} m(x) e^{-\lambda_\alpha a^\alpha(x)}.
\end{equation}
The corresponding entropy is
\begin{equation}
  S(A) = \log Z(\lambda) + \lambda_\alpha A^\alpha,
\end{equation}
with $\lambda_\alpha$ and $Z(\lambda)$ given by Eq.(10). Analogous expressions hold for the primed quantities. The formalism simplifies considerably when the bath is large enough that exchanges of $A$ do not affect it, and $\lambda'$ remains fixed at $\lambda_0$. Then
\begin{equation}
  S'(A_T - A) = \log Z'(\lambda_0) + \lambda_0 A^\alpha = \text{const} - \lambda_0 A^\alpha. \quad (15)
\end{equation}

The probability that the value of $A$ fluctuates into a small volume $g^{1/2}(A)dA$ is given by our main result Eq.(10),
\begin{equation}
  \pi(A)dA = \frac{1}{\zeta(\lambda_0)} e^{S(A) - \lambda_0 A^\alpha} g^{1/2}(A)dA \quad \text{where} \quad g_{\alpha\beta} = -\frac{\partial^2 S(A)}{\partial A^\alpha \partial A^\beta},
\end{equation}
and $\zeta(\lambda_0)$ is a suitably defined normalization. To the extent that the right choice of variables has been made, Eq.(16) is exact.

An important difference with the usual theory stems from the presence of the Jacobian factor $g^{1/2}(A)$. This is required by coordinate invariance and can lead to small deviations from the canonical predictions. The quantities $\langle \lambda_\alpha \rangle$ and $\langle A^\alpha \rangle$ may be close but will not in general coincide with the quantities $\lambda_0$ and $A_0^\alpha$ at the point where the scalar probability density attains its maximum. When this maximum is very sharp and in its vicinity the Jacobian can be considered constant the usual results follow. The remaining difficulties are purely computational and of the kind that can in general be tackled systematically using the method of steepest descent to evaluate the appropriate generating function.

Since we are not interested in variables referring to the bath we can integrate Eq.(12) over $x'$, and use the distribution $p(x,A) = \pi(A)p(x|A)$ to compute various moments. As an example, the correlation between $\delta \lambda_\alpha = \lambda_\alpha - \langle \lambda_\alpha \rangle$ and $\delta A^\beta = a^\beta - \langle A^\beta \rangle$ or $\delta A^\beta = A^\beta - \langle A^\beta \rangle$ is
\begin{equation}
  \langle \delta \lambda_\alpha \delta A^\beta \rangle = -\frac{\partial \langle \lambda_\alpha \rangle}{\partial \lambda_\beta} + (\lambda_0 - \langle \lambda_\alpha \rangle) \left( A_0^\beta - \langle A^\beta \rangle \right). \quad (17)
\end{equation}
When the differences $\lambda_0 - \langle \lambda_\alpha \rangle$ or $A_0^\beta - \langle A^\beta \rangle$ are negligible one obtains the usual expression, $\langle \delta \lambda_\alpha \delta a^\beta \rangle \approx -\delta^\beta \lambda_\alpha$. 


5 Entropic priors

The last problem we address is that of obtaining a prior $\pi(\theta)$ for use in Bayes’ theorem, $p(\theta|x) \propto \pi(\theta)p(x|\theta)$. The traditional approach has been to attempt to determine or at least to constrain $\pi(\theta)$ by requiring that it be non-informative, that it satisfy coordinate invariance, and so on. The seemingly innocuous but fruitful new idea proposed by Rodríguez [13] is to focus attention on $p(x, \theta)$ instead of $\pi(\theta)$. One could well wonder whether this makes any difference. After all, once $p(x|\theta)$ is known, $p(x, \theta)$ can be calculated from $\pi(\theta)$ and vice versa.

It makes a huge difference. The selection of a preferred distribution using the ME method demands that one specify in which space the search will be conducted. Being a consequence of the product rule, Bayes’ theorem requires that $p(x, \theta)$ be defined and that assertions such as “$x$ and $\theta$” be meaningful. The relevant universe of discourse is neither $X$ nor $\Theta$, but the product $X \times \Theta$.

The complete specification of the space $X \times \Theta$ requires a measure $m(x, \theta)$. At this point we do not know anything about the variables $\theta$, they are totally arbitrary. To the extent that no relation between $x$ and $\theta$ is known, the measure must be the product $m(x)\mu(\theta)$ of the separate measures in the spaces $X$ and $\Theta$. Indeed, the distribution that maximizes

$$\sigma[p] = -\int dx \, d\theta \, p(x, \theta) \log \frac{p(x, \theta)}{m(x)\mu(\theta)},$$

is $p(x, \theta) \propto m(x)\mu(\theta)$; it is such that data about $x$ tells us nothing about $\theta$. In what follows we assume that $m(x)$ is known; this is part of understanding what data it is that has been collected. The measure $\mu(\theta)$ remains undetermined.

Next we incorporate the crucial piece of information: in order to infer something about $\theta$ on the basis of a measurement of $x$, a relation between $x$ and $\theta$ must exist. The relation is supplied by the model $p(x|\theta)$. This constrains the joint distribution $p(x, \theta)$ to be of the form $\pi(\theta)p(x|\theta)$ and removes the ambiguity in the choice of $\mu(\theta)$. As mentioned before, there is a natural choice $\mu(\theta) = g^{1/2}(\theta)$, where $g(\theta)$ is the determinant of the Fisher-Rao metric $g_{ij}$. Having identified the space, the measure, and the constraints, the ME method gives the probability $\pi(\theta)$ that the value of $\theta$ should lie within the small volume $g^{1/2}(\theta)d\theta$. It is our previous main result, Eq.(10),

$$\pi(\theta)d\theta \propto e^{S(\theta)}g^{1/2}(\theta)d\theta.$$

(19)

It is remarkable that the ingredients that have been used are precisely those that led us to consider using Bayes’ theorem in the first place. Once the model is known, which means that the data space $X$, its measure $m(x)$, and the conditional distribution $p(x|\theta)$ are given, the prior probability $\pi(\theta)$ is unambiguously determined.

We emphasize that $\pi(\theta)$ in Eq.(19) is not the least informative distribution, it is the distribution after we learn $p(x|\theta)$. The distribution before we learn $p(x|\theta)$ is $\mu(\theta)$. We do not know it; this is truly noninformative.
No doubt the reader recognizes that essentially the same argument has been given twice, first in Sect. 3 and then here. There is a reason for this repetition. It was not a priori obvious (at least to this author) that there could have existed a relation between, say, the theory of thermodynamic fluctuations and the problem of selecting priors in Bayesian inference. They are most definitely not the same problem; the meanings of the various symbols and the motivations driving our interests in these questions do not coincide. It was therefore not at all clear that exactly the same mathematical formalism could provide the solution to both. Two verbal justifications, rather than just one, were needed.

The prior $\pi(\theta)$ in Eq. (19) is a member of the family of distributions labelled by the real parameter $\alpha$,

$$\pi(\theta, \alpha) = \frac{1}{\zeta(\alpha)} e^{\alpha S(\theta)} g^{1/2}(\theta), \quad \zeta(\alpha) = \int d\theta g^{1/2}(\theta) e^{\alpha S(\theta)},$$  \hspace{1cm} (20)

which are known as entropic priors [13]-[15]. The ME approach has unambiguously selected the $\alpha = 1$ member. Indeed, it is easy to check that values $\alpha \neq 1$ do not maximize the $\sigma$ entropy, $\sigma[\pi(\theta, 1 + \varepsilon)] \leq \sigma[\pi(\theta, 1)]$.

The $\alpha = 1$ entropic prior has, in the past, led to manifestly reasonable results. Examples include the entropic prior for the family of Gaussians [15], and the distribution dual to the Maxwell-Boltzmann distribution [7]. The justifications given for these two cases are totally independent of each other and of ours; both are instances of Jeffreys’ prior for scale parameters [11]. On the other hand, values $\alpha \neq 1$ have also been used. To investigate this further we consider experiments that can be repeated.

Experiments need not be repeatable. Assume, however, that successive repetitions are possible and that they happen to be independent. Suppose, to be specific, that the experiment is performed twice so that the space of data $X \times X = X^2$ consists of the possible outcomes $x_1$ and $x_2$. Suppose further that $\theta$ is not a “random” variable; the value of $\theta$ is fixed but unknown. Then the joint distribution in the space $X^2 \times \Theta$ is

$$p(x_1, x_2, \theta) = \pi(2)(\theta) p(x_1, x_2|\theta) = \pi(2)(\theta)p(x_1|\theta)p(x_2|\theta),$$  \hspace{1cm} (21)

and the appropriate $\sigma$ entropy is

$$\sigma(2)[\pi] = - \int dx_1 dx_2 d\theta p(x_1, x_2, \theta) \log \frac{p(x_1, x_2, \theta)}{\sqrt{g^{(2)}(\theta)} m(x_1)m(x_2)},$$  \hspace{1cm} (22)

where $g^{(2)}(\theta)$ is the determinant of the Fisher-Rao metric for $p(x_1, x_2|\theta)$. From Eq. (6) it follows that $g_{ij}^{(2)} = 2g_{ij}$ so that $g^{(2)}(\theta) = 2^d g(\theta)$, $d$ being the dimension of $\theta$. Maximizing $\sigma(2)[\pi]$ subject to $\int d\theta \pi(2)(\theta) = 1$ we get

$$\pi(2)(\theta) = \frac{1}{Z(2)} g^{1/2}(\theta) e^{S(2)(\theta)} = \frac{1}{Z(2)} g^{1/2}(\theta) e^{2S(1)(\theta)},$$  \hspace{1cm} (23)

where $S(2)(\theta) = 2S(1)(\theta) \equiv 2S(\theta)$ is the entropy of $p(x_1, x_2|\theta)$. The generalization to $n$ repetitions of the experiment, with data space $X^n$, is immediate: the
ME prior $\pi^{(n)}(\theta)$ is obtained replacing $S^{(2)}(\theta)$ with $S^{(n)}(\theta) = nS^{(1)}(\theta)$. The coefficient in front of $S^{(n)}(\theta)$ remains $\alpha = 1$ and the prior $\pi^{(n)}(\theta)$ differs from $\pi^{(1)}(\theta)$. This is puzzling. Do we have to revise our prior as more data comes in? In fact, for large $n$ the prior $\pi^{(n)}(\theta)$ above becomes manifestly wrong: the exponential preference for the value of $\theta$ that maximizes $S^{(1)}(\theta)$ becomes so pronounced that no amount of data to the contrary can successfully overcome its effect.

Repeatable experiments present us with a problem, but how do we deny preferred status to $\alpha = 1$ without simultaneously challenging the ME principle itself? There is one way out of this dilemma. Readers of Jaynes’ work will surely recognize the following argument: we have been conducting our search with the wrong constraint. There is something we know about repeatable experiments that we have not incorporated into the ME procedure above. I propose it is this: when we say an experiment can be repeated say, twice, $n = 2$, we actually know more than just $p(x_1, x_2 | \theta) = p(x_1 | \theta)p(x_2 | \theta)$. We also know that forgetting or discarding the value of say $x_2$, yields an experiment that is totally indistinguishable from the single, $n = 1$, experiment. This additional information is quantitively expressed by the constraint $\int dx_2 p(x_1, x_2, \theta) = p(x_1, \theta)$, or equivalently

$$\int dx_2 \pi^{(2)}(\theta)p(x_1|\theta)p(x_2|\theta) = \pi^{(1)}(\theta)p(x_1|\theta),$$

which leads to $\pi^{(2)}(\theta) = \pi^{(1)}(\theta)$. In the general case we get the manifestly reasonable result $\pi^{(n)}(\theta) = \pi^{(n-1)}(\theta) = \ldots = \pi^{(1)}(\theta)$; the undesired dependence on $n$ has been eliminated.

The conclusion is that our result Eq. (19) stands: $\alpha = 1$ is the default value. Unless there is positive evidence to the contrary, the entropic prior with $\alpha = 1$ should be preferred. But, of course, the results of Sect. 3 apply here too. The preference for maximum entropy is not absolute: $\alpha = 1$ is just the maximum $\sigma$ distribution, and values of $\alpha$ corresponding to less than maximum $\sigma$ are not totally ruled out.

6 Final remarks

The method of maximum entropy has been extended to give a quantitative determination of the degree to which distributions with lower entropy are ruled out. The same idea was used to extend the theory of thermodynamic fluctuations and in the construction of priors for Bayesian inference. That a connection between these two historically independent topics should at all exist is in itself quite remarkable.

We conclude with a comment on the reliability of using entropy as a tool for reasoning. There are several reasons why the ME method could lead to an absurd answer. One possibility is that there is relevant prior information that remains unidentified. Another possible reason for failure is a wrong choice of variables. Choosing the right variables is perhaps the most serious difficulty
in statistical mechanics; in fact, it takes many years of indoctrination before it is obvious that the Cooper pair wave function is the right variable to describe superconductivity.

These two possibilities, failure to identify the correct constraints or to identify the correct variables, do not reflect a flaw of the ME method itself. Of course, it is conceivable, that it is the ME axioms that fail, or that real numbers are not the right way to measure entropy, or even worse, that there is no universal set of rules for processing information. But one need not be overly cautious in this last respect. It is clear that the ME method is applicable to a vast range of problems, and at this point, there are absolutely no signs that the exploration of this territory is anywhere near completion.

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