MAXIMUM ENTROPY MULTIVARIATE DENSITY ESTIMATION: 
AN EXACT GOODNESS-OF-FIT APPROACH

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ABSTRACT
We consider the problem of estimating the population probability distribution 
given a finite set of multivariate samples, using the maximum entropy approach. 
In strict keeping with Jaynes' original definition, our precise formulation of the 
problem considers contributions only from the smoothness of the estimated distri- 
bution (as measured by its entropy) and the loss functional associated with 
its goodness-of-fit to the sample data, and in particular does not make use of 
any additional constraints that cannot be justified from the sample data alone. 
By mapping the general multivariate problem to a tractable univariate one, we 
are able to write down exact expressions for the goodness-of-fit of an arbitrary 
multivariate distribution to any given set of samples using both the traditional 
likelihood-based approach and a rigorous information-theoretic approach, thus 
solving a long-standing problem. As a corollary we also give an exact solution 
to the ‘forward problem’ of determining the expected distributions of samples 
taken from a population with known probability distribution.

1. Introduction

According to Jaynes1, the maximum entropy distribution is “uniquely determined 
as the one which is maximally noncommittal with regard to missing information, in 
that it agrees with what is known, but expresses maximum uncertainty with respect 
to all other matters”2.

On the other hand, Kapur and Kesavan3 state that “the maximum entropy dis- 
bution is the most unbiased distribution that agrees with given moment constraints 
because any deviation from maximum entropy will imply a bias”.

While the latter neatly encapsulates the modern interpretation of the maximum 
entropy principle in its application to density estimation, it is not equivalent to the 
definition given by Jaynes as it restricts its use to the case where the moments of the 
population distribution are already known.

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While this restriction may be convenient, it is not valid in any case in which one is not simply trying to re-derive a standard distribution based upon its known moments using maximum entropy principles. Rather, in practical applications the moments of the population distribution are not (and indeed cannot) be known a priori, and certainly cannot be determined on the basis of a finite number of samples.

In this paper, we give an explicit and exact expression of the maximum entropy density estimation problem in a form which is strictly in keeping with Jaynes’ original (and precise) definition.

2. Reformulating the MaxEnt Problem

So let us return to basics and consider the problem of estimating the multivariate population density distribution given a finite set of samples taken at random from the population, assuming that the raw sample data is the only prior information we have. In this case, which is clearly of the most general practical applicability, the requirement that the maximum entropy distribution ‘agrees with what is known’ is equivalent to the requirement that the population distribution provides a good fit to the sample data. In this sense the maximum entropy distribution can be defined as “the distribution of maximum entropy subject to the provision of a good fit to the sample data”, with the only potential uncertainty lying in the relative importance which should be attached to each of the two contributions. While this uncertainty reflects the supposed ill-posedness of the density estimation problem, Jaynes’ definition implies that there should in fact exist a unique solution, so that even this uncertainty is in principle resolvable. While we do attempt to resolve this issue here, the matter certainly deserves further attention.

The definition given in the last paragraph allows us to formulate the maximum entropy multivariate density estimation problem in precise mathematical terms. If we denote the estimated distribution by \( f(r) \) where \( r \in \mathbb{R}^D \), and the sample data set by \( \{x_1, \ldots, x_N\} \), we would like to maximise the functional defined by,

\[
F[f(r)] = S[f(r)] + \alpha G[f(r), \{x_i\}],
\]

where \( S[f(r)] \) is the normalised\(^a\), sample-independent entropy of the estimated distribution over its domain of definition,

\[
S[f(r)] = -\frac{1}{\log V} \int f(r) \log f(r) \, d\tau,
\]

and \( G[f(r), \{x_i\}] \) is a precise measure of the goodness-of-fit of the distribution to the sample data. An optional tunable variable \( \alpha \in [0, \infty] \) has been included which parametrises the solutions. It is clear by inspection that \( \alpha = 0 \) implies the sample-independent maximum entropy solution represented by the uniform distribution \( f(r) = \)

\(^a\)The normalisation factor is fixed by requiring that the entropy of the uniform distribution be unity.
constant, while the limit $\alpha \to \infty$ corresponds to the distribution providing the best fit to the data without regard to its entropy. The solution for any other value of $\alpha$ will represent some trade-off between maximising entropy and maximising the goodness-of-fit. The fact that neither of the two extremal solutions would be of use in practical applications does support the argument that there should exist an optimal value for $\alpha$ (presumably unity), and hence a unique optimal density estimate. We will come back to this point later.

3. Establishing the Goodness-of-Fit

We have yet to give the expression for the goodness-of-fit $G[f(r), \{x_i\}]$. In the absence of an analytically rigorous and generally applicable measure of goodness-of-fit, various ad hoc schemes have been used in the past\textsuperscript{4,5}. As we will show, there do exist unique analytical expressions for the goodness-of-fit of an arbitrary multivariate probability distribution $f(r)$ to a given set of sample data $\{x_1, \ldots, x_N\}$ depending on whether a likelihood-based or information-theoretic approach is used. While the former does correctly provide the likelihood of obtaining any particular set of sample values assuming a given population distribution, we will nevertheless demonstrate that it is the information-theoretic approach that is the appropriate one to use to find the population distribution which best accounts for the samples observed.

3.1. Mapping Multivariate Estimation to a Univariate Problem

It happens that there exists a well-defined procedure for mapping the complex multivariate problem into a tractable univariate one. To proceed, one needs to note that the probability of a sample taking values in a particular region of $R^D$ is given by the area (or more generally the hypervolume) under the curve $f(r)$ over that region. Moreover we know that for a probability distribution, the total area under the curve is normalised to unity.

The key step is to define a mapping $C_f : R^D \rightarrow I$ (representing a particular kind of cumulative probability density function corresponding to $f(r)$) from $R^D$ onto the real line segment $I = [0, 1]$ as follows,

$$C_f(x) = \int f(r)\Theta[f(x) - f(r)]d\tau,$$  \hspace{1cm} (3)

where $x \in R^D$ and $\Theta(y)$ is the Heaviside step function with $\Theta(y) = 1$ for $y \geq 0$ and $\Theta(y) = 0$ otherwise. The mapping $C_f$ will in general be many-to-one. Its utility lies in the fact that if we take the set of samples $\{x_1, \ldots, x_N\}$ in $R^D$ and map them to the the set of points $\{C_f(x_1), \ldots, C_f(x_N)\}$ on the segment $I$ then, in view of the equivalence between the probability and the area under the curve, the goodness-of-fit of $f(r)$ to the samples $\{x_i\}$ is precisely equal to the goodness-of-fit of the uniform probability distribution $g(x) = 1$ defined on the segment $I$ to the mapped samples.
{C_f(x_i)}. Let us now consider the latter case in more detail.

3.2. Uniformly Distributed Samples on a Real Line Segment

Consider a perfect random number generator which generates values uniformly distributed in the range \([0, 1]\). Suppose we plan to use it to generate \(N\) random samples. We can calculate in advance the probability distribution \(p_{N,i}(x)\) of the \(i\)-th sample (where the samples are labelled in order of increasing magnitude), as follows.

Let \(X_i\) be the random variable corresponding to the value of the \(i\)-th sample for each \(i = 1 \ldots N\). Note that the probability of a number (selected at random from \([0, 1]\) assuming a uniform distribution) being less than some value \(x \in [0, 1]\) is simply \(x\), while the probability of it being greater than \(x\) is \(1 - x\). Thus, if we consider the \(i\)-th value in a set of \(N\) samples taken at random, the probability that \(X_i\) takes the value \(x\) is given by the product of the probability \(x^{i-1}\) that \(i - 1\) of the values are less than \(x\) and the probability \((1 - x)^{N-i}\) that the remaining \(N - i\) values are greater than \(x\), divided by a combinatorial factor \(Z_{N,i}\) counting the number of ways \(N\) integers can be partitioned into three sets of size \(i - 1\), 1 and \(N - i\) respectively,

\[
p_{N,i}(x) \equiv P(X_i = x) = Z_{N,i}^{-1}x^{i-1}(1-x)^{N-i}. \tag{4}
\]

From simple combinatorics, the value of \(Z_{N,i}\) is given by,

\[
Z_{N,i} = \frac{N!}{(i-1)!(N-i)!} = \frac{\Gamma(N+1)}{\Gamma(i)\Gamma(N-i+1)} = B^{-1}(N-i+1,i), \tag{5}
\]

where \(B(p, q)\) is the Euler beta function which appears in the Veneziano amplitude for string scattering\(^6\). That this value is correct can be checked using the fact that \(p_{N,i}(x)\) must be normalised so that \(\int p_{N,i}(x)dx = 1\), and noting that the resulting integral is just the definition of the beta function given above. Note also that if experiments are carried out in which sets of \(N\) samples are taken repeatedly, the expectation of the \(i\)-th sample is given by,

\[
E[X_i] = \int_0^1 xp_{N,i}(x)dx = \frac{i}{N+1}, \tag{6}
\]

for \(i = 1 \ldots N\), corresponding to the most regularly distributed configuration of the \(N\) samples possible, and in excellent accord with intuition.

3.3. The Maximum Likelihood Approach

Taking a traditional likelihood-based approach, an expression for the goodness-of-fit of a set of \(N\) samples to the uniform distribution on \([0, 1]\) can now be obtained by first labelling the samples in order of increasing magnitude and then calculating the likelihood given by,
\[ L[\{x_i\}] = \prod_{i=1}^{N} p_{N,i}(x_i). \]  

Bearing in mind the mapping \( C_f : R^D \rightarrow I \) defined in (3), we can generalise the above to derive an exact expression for the goodness-of-fit of a set of \( N \) samples \( \{x_1, \ldots, x_N\} \) to an arbitrary multivariate probability distribution \( f(r) \),

\[ L[f(r), \{x_i\}] = L[\{C_f(x_i)\}] = \prod_{i=1}^{N} p_{N,i}(C_f(x_i)). \]  

where the samples are now labelled in order of increasing magnitude of \( f(x_i) \) and hence \( C_f(x_i) \).

Let us take a closer look at the likelihood measure of Eqn.(7) and in particular, let us consider the simple illustrative case when only two samples are taken from the uniform distribution on \([0,1]\). In this case, the likelihood is maximised if the samples happen to take precisely the values 0 and 1. This slightly perturbing result is actually correct and is one of the reasons why care must be taken if one wishes to apply likelihood-based arguments in the opposite direction to estimate the population distribution based upon observed sample data. More generally, the expression (8) for the likelihood will always be biased towards the case where the position of the first sample coincides with the minimum value of the probability distribution and that of the last sample with its maximum.

These considerations are sufficient to show that the maximum likelihood approach to multivariate density estimation is problematic and provide us with good reason to seek an alternative, more rigorous approach.

3.4. The Information Theoretic Approach

The rigorous alternative lies in taking an information theoretic approach. Indeed we will show that it is possible to assign a unique entropy associated with the goodness-of-fit of the estimated population distribution to the sample data in the same way (see Eqn.(2)) that an entropy was assigned to the estimated distribution itself.

To see how, consider the values \( y_i \equiv C_f(x_i) \) of the samples obtained after having mapped them to the real segment using the mapping defined in Eqn.(3). Defining \( y_0 = 0 \) and \( y_{N+1} = 1 \) for convenience, these values are constrained by the ‘normalisation’ property,

\[ \sum_{i=1}^{N+1} y_i - y_{i-1} = 1. \]  

Then by considering each of the \( N+1 \) gaps between the values as ‘sample bins’, and the size \( d_i \equiv y_i - y_{i-1} \) of each gap as the probability associated with the corresponding
bin, it becomes possible to identify the distribution of the mapped samples on $[0, 1]$ with a discrete probability distribution defined over the set of $N + 1$ sample bins. The (normalised) entropy associated with the fit of the estimated population distribution to the sample data can then be equated with the entropy of the equivalent discrete probability distribution,

$$S'[f(r), \{x_i\}] \equiv -\frac{1}{\log(N + 1)} \sum_{i=1}^{N+1} d_i \log d_i.$$  \hfill (10)

This is just the discrete version of the expression given in Eqn.(2) for a continuous probability distribution. Maximising Eqn.(10) for the entropy results immediately in the desirable property that the samples are equally spaced, namely $y_i = i/(N + 1)$, in agreement with the expected values obtained less directly in Eqn.(6).

The discussion above strongly suggests that the entropy $S'$ of Eqn.(10) should be used instead of the traditional likelihood (as given here by Eqn.(8)), both as a measure of the goodness-of-fit of an arbitrary population distribution to a given set of multivariate samples, and also as the second term $G[f(r), \{x_i\}]$ appearing in the functional of Eqn.(1).

Substituting (10) into (1), we claim that the rigorous solution to the MaxEnt multivariate density estimation problem is given by the probability distribution which maximises the functional,

$$F[f(r)] = -\frac{1}{\log V} \int f(r) \log f(r) d\tau - \frac{\alpha}{\log(N + 1)} \sum_{i=1}^{N+1} d_i \log d_i,$$  \hfill (11)

where,

$$d_i = C_f(x_i) - C_f(x_{i-1}),$$  \hfill (12)

and the mapping $C_f$ is given by Eqn.(3). In (11) the parameter $\alpha \in [0, \infty]$ can be used to tune the solutions, bearing in mind that a smaller value will emphasise the smoothness of the resulting distribution, while a larger value will emphasise the goodness of fit. Setting $\alpha$ to unity and maximising will in principle give the unique maximum entropy distribution as originally envisioned by Jaynes\textsuperscript{c}.

The information-theoretic approach we have described in this section is more rigorous and compelling than the traditional likelihood approach, as clearly evidenced by the pleasingly symmetric form (11) of the resulting optimisation problem. In\textsuperscript{b}Note that there is some potential for non-uniqueness to creep in due to the possibility of degenerate solutions in certain situations such as when $N$ is very small or when the samples are distributed highly symmetrically.

\textsuperscript{c}The fact that the entropy of a uniform distribution over $[-\infty, \infty]$ is infinite ($\sim \log V$), while being finite for other distributions ($\sim \log \sigma \sqrt{2\pi e}$ for a univariate Gaussian), suggests that special attention may be required in the non-compact case to prevent one term overwhelming the other. A simple way of regulating the problem is to consider non-compact domains as extremal limits of compact ones where the distributions are constrained to be smooth and to vanish at the boundaries.
particular, both terms contributing to the functional are associated with entropies - the first term being the entropy associated with the smoothness of the estimated population distribution, and the second term being the entropy associated with the goodness-of-fit of the distribution to the sample data.

Algorithms implementing the optimisation procedure are under development, which will allow us to calculate specific solutions of (11) and to perform more detailed investigations of their properties. We hope to present these results in a future paper.

3.5. A Corollary: The Forward Problem

Before ending, it is worth mentioning here as a corollary that the distributions $p_{N,i}(x)$ of (4) also help us to solve the ‘forward problem’, i.e. that of determining the expected distributions $p_{N,i}^f(r)$ of any set of $N$ samples taken at random from a multivariate population where the population density distribution $f(r)$ is given.

3.5.1. The univariate case

We would like to know the expected distribution of the samples when the univariate population distribution $f(x)$ is given. In place of the mapping of (3), it is appropriate here to consider the mapping $C_f'$ defined by the cumulative probability density function,

$$C_f'(x) = \int_{-\infty}^{x} f(y) \, dy.$$  \hfill (13)

If the univariate samples are labelled in increasing order of value then their expected distributions are given by,

$$p_{N,i}^f(x) = p_{N,i}(C_f'(x)),$$  \hfill (14)

and these can be used for example to estimate the experimental errors in individual sample values given an estimate of the population distribution\(^7\).

3.5.2. The multivariate case

The forward problem does not have an obvious generalisation to the multivariate case because of the lack of an unambiguous definition of the cumulative probability density function in that case. Nevertheless we can instead apply the mapping $C_f$ of Eqn.(3) (paying careful attention to the degeneracies present) to obtain the following expected distributions for the samples ordered as described below Eqn.(8),

$$p_{N,i}^f(r) = J^{-1}(r) p_{N,i}(C_f(r)),$$  \hfill (15)
where $J(r)$ measures the (typically $(D - 1)$-dimensional) volume of the degeneracy of $f(r)$ (i.e. the volume of the subspace of $R^D$ sharing the same value of $f(r)$) for each value of $r$. At special values the region of degeneracy may have dimensionality less than $(D - 1)$ in which case the value of $p_{N,i}^f(r)$ becomes irrelevant and can safely be ignored. On the other hand for distributions which contain $D$-dimensional subspaces throughout which $f(r)$ is constant (the uniform distribution being an obvious example), then special considerations will be required in order to generalise the analysis leading to Eqn.(4) for the real line segment to irregular, multidimensional, and possibly non-compact spaces. Excepting the simplest cases, such an analysis promises to be highly non-trivial and we will not attempt to delve into such intricacies here. Note that (15) does not agree with (14) in the univariate case as the labelling of the samples and the corresponding interpretations of the distributions are quite different in each case.

It is often assumed that the deviations of individual observations from their expected values follow a normal distribution for univariate data, leading to a $\chi^2$ measure of goodness-of-fit. Our exact results in Eqn.(14) demonstrate that this approximation only holds if $N$ is sufficiently large and only then if $f(r)$ is sufficiently well-behaved. We will conclude our analysis at this point.

4. Summary and Discussion

The purpose of the present work has been to reformulate the maximum entropy (MaxEnt) density estimation problem in a precise way which is in strict keeping with its original definition as introduced by Jaynes. The importance of having such a precise formulation hardly needs mentioning given the ubiquity of the estimation problem throughout the sciences.

In reaching our formulation we have managed to solve the long-standing problem of obtaining an exact expression for the likelihood of observing any particular set of sample values when taken at random from a given population. This is useful in the experimental sciences for validating theoretical models on the basis of observations. As a corollary, we have also been able to propose the solution to the ‘forward problem’ - that of determining the distribution of the samples when the population distribution is known.

The traditional maximum likelihood approach was shown to have some unsatisfactory features when applied to the problem of density estimation. On the other hand, by taking a novel information-theoretic approach we have succeeded in deriving an explicit and rigorous entropic measure of the goodness-of-fit of a generic population distribution to a given set of multivariate samples. This in turn has made it possible to reformulate the MaxEnt density estimation problem in a unique, precise and

\[^d\text{A discussion of the trade-off between smoothness and goodness-of-fit in the context of this assumption appears in Gull (1989).}\]
purely information-theoretic way.

We have made allowance for the introduction of an optional tunable parameter in our expression of the MaxEnt problem which parametrises solutions ranging from those with maximal smoothness to those providing maximal fit to the data. The effect of this parameter on the solutions has not been discussed in detail here, and we intend to come back to it in future once computational algorithms implementing the optimisation have been developed.

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6. References

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