What is the question that MaxEnt answers?

A probabilistic interpretation

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Abstract. The Boltzmann-Wallis-Jaynes' multiplicity argument is taken up and elaborated. MaxEnt is proved and demonstrated to be just an asymptotic case of looking for such a vector of absolute frequencies in a feasible set, which has maximal probability of being generated by a uniform prior generator/pmf.

Keywords: prior generator, occurrence vector, constraints, minimum I-divergence, minimum J-divergence, linear inverse problem, Shannon’s entropy, MaxEnt

Abbreviations: MaxEnt – Maximum Entropy method, REM – Relative Entropy Maximization, MaxProb – Maximum Probability method, ExpOc – Expected Occurrence vector method

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1. Introduction

Shannon’s entropy maximization (MaxEnt) interpreted by its proponent, E.T. Jaynes, as a ‘method for inference from incomplete information’ (Jaynes, 1991), has a debatable relationship to the Bayesian method (see (Jaynes, 1988), (Zellner, 1988), (Seidenfeld, 1987), (Uffink, 1995), (Golan, Judge and Miller, 1996)), and to the Maximum Likelihood method (see (Jaynes, 1982), (Golan, 1998), (Mohammad-Djafari, 1998), (Grendar and Grendar, 1999)). MaxEnt has also been presented as a method for assigning prior probabilities (see (Jaynes, 1998)), ((Seidenfeld, 1987), (Uffink, 1995) for a critique), and as an extension of the principle of insufficient reason. On the theoretical level MaxEnt, as a statistical method, is in dispute for decades.

MaxEnt has been successfully applied to linear inverse problems without noise that arise in many branches of science. Its scope was substantially extended to the inverse problems with noise by (Golan, Judge and Miller, 1996), and further by (van Akkeren and Judge, 1999), (Mittelhammer, Judge and Miller, 2000), who have put MaxEnt into a context of extremum estimation and inference methods.
Theoretical disputes on the status of MaxEnt among other statistical methods generally ignore a fundamental question: 'What is the question MaxEnt answers?'. Two other problems involving 'What kind of constraints are relevant to bind the entropy maximization?' and 'What if information on amount of data is also available?' considerations were left on margin of interest both by Jaynes and opponents of MaxEnt.

In this article we address three elementary problems of the MaxEnt method. These problems involve lack of satisfactory probabilistic rationale, ad-hockery regarding constraints to bind MaxEnt and impossibility of the method to take an information on amount of data into consideration.

Concerning the problem of rationale, we shall prove and demonstrate that MaxEnt is a special, asymptotic case of more general and self-evident 'principle/method' – MaxProb – that focuses on looking for a vector of absolute frequencies (occurrences) in a feasible set of vectors, which has maximal probability of being generated by a prior generator pmf. MaxEnt is also a special case of MaxProb in the sense of assuming a specific uniform pmf prior generator. In fact, the work provides probabilistic rationale of a more general, relative entropy maximization (REM) method. REM is also commonly known as $I$-divergence minimization, or Kullback-Leibler directed distance minimization. As a by-product of providing the MaxProb rationale of MaxEnt, the remaining two problems concerning the issues of relevant constraints and the known-sample-size are also resolved.

The article is organized as follows: Section 2 reviews an up-to-date status of work on the three above mentioned problems. Section 3 introduces MaxProb and states the main Theorem 1 together with an example illustrating the point. Section 4 summarizes briefly consequences of Theorem 1 for MaxEnt. Proof of the Theorem is given in Appendix A. Appendix B contains a bonus.

2. Three MaxEnt problems

We start with a brief review of three problems pertaining to MaxEnt.

MaxEnt, in the realm of statistics, lacks a proper rationale. Moment based probability distribution recovered through Shannon’s entropy maximization have been characterized as the smoothest, the flattest, the most uniform given a constraints, the least prejudiced, the one that maximizes our ignorance while including the available statistical data. These adjectives usually serve as the main rationale for employing Shannon’s entropy criterion. Rarely, two justifications Jaynes had developed are recalled. The first one, Wallis’ multiplicity argument, is
presented in Chapter 11 of (Jaynes, 1998). We give it form of theorem and highlight the central role played by Jaynes’ limiting process.

**Wallis–Jaynes Theorem.** Let \( N \) be a discrete multivariate \( m \)-dimensional random variable from multinomial distribution

\[
P(N = n) = \pi(n|q) = \frac{n!}{n_1! n_2! \ldots n_m!} \prod_{i=1}^{m} q_i^{n_i}
\]

where \( \sum_{i=1}^{m} n_i = n \), and \( q = [1/m, 1/m, \ldots, 1/m]^t \) is uniform.

Then under Jaynes’ limiting process

1) \( n \to \infty \)
2) \( n_i \to \infty \) for \( i = 1, 2, \ldots, m \)
3) \( n_i/n \to p_i \), where \( p_i \) is a constant, for \( i = 1, 2, \ldots, m \),

holds

\[
\frac{\ln \pi(n|q)}{n} \to H(p)
\]

where \( H(p) = -\sum_{i=1}^{m} p_i \ln p_i \) is Shannon’s entropy (up to an additive constant, \( -\ln m \)).

**Proof.** Due to Stirling’s formula (there is a typo at the Stirling’s approximation (see formula (11-17)) in the Jaynes’ book)

\[
\ln n! = n \ln n - n + \ln(\sqrt{2\pi n}) + 1/(12n) + O(1/n^2)
\]

holds

\[
\ln \pi(n|q) = n \ln n - n + \ln(\sqrt{2\pi n}) + 1/(12n) - \sum_{i=1}^{m} n_i \ln n_i - \sum_{i=1}^{m} \ln(\sqrt{2\pi n_i}) - \sum_{i=1}^{m} 1/(12n_i)
\]

\[
+ \sum_{i=1}^{m} n_i \ln q_i + O(1/n^2)
\]

Taking into account that \( \sum_{i=1}^{m} n_i = n \), and the first two assumptions of the Jaynes’ limiting process give

\[
\frac{\ln \pi(n|q)}{n} \to \ln n - (1/n) \sum_{i=1}^{m} n_i \ln n_i - \ln m
\]

where the RHS is \( -\sum_{i=1}^{m} \frac{n_i}{n} \ln \frac{n_i}{n} - \ln m \), which leads thanks to the third assumption of the limiting process to the claim of the Theorem. \( \square \)
In order to provide a rationale for Shannon’s entropy maximization one has to investigate each particular set of constraints binding maximization of $\pi(n|q)$ to determine whether the constraints induce just the Jaynes’ limiting process. Yet it has not been done, and it seems to be not the case, even for the simplest, moment consistency constraints (mcc), traditionally accompanying the entropy maximization. For, even in the case of mcc, there is for any $n$ at least one vector $n$ in conflict with the second requirement of Jaynes’ limiting process.

Thus, Wallis’ argument, rather than offering explanation of MaxEnt, presents yet another (and interesting) partial limit of multinomial distribution, in addition to the well-known DeMoivre-Laplace and the Poisson one. It could be better called ‘Wallis-Jaynes local limit theorem’.

The second rationale, Jaynes proposed has been dubbed ‘The Entropy Concentration Theorem’, (see (Jaynes, 1979), (Jaynes, 1982), or (Seidenfeld, 1987)). This rationale rests on the Wallis’ argument and Jaynes’ limiting process and again leads to the question about its relevance to constraints bound entropy maximization.

It is well known that MaxEnt can not incorporate information on amount of data (see for instance (Uffink, 1996)), or in other words, MaxEnt recovers the same pmf regardless of the sample size. This second problem of MaxEnt, is usually left open, although it directly relates to the next, more frequently debated, third problem concerning the kind of constraints relevant to bind the entropy maximization. According to (Jaynes, 1979), constraints should represent testable information, i.e. they should be a test basis concerning the probability distribution. For instance a set of samples is not testable, value of, let’s say, third moment is. Such a state of art also reveals lack of internal coherence of the views on entropy maximization.

Three interconnected questions are ‘Just what are we accomplishing when we maximize entropy?’ (Jaynes, 1982), ‘What kind of constraints are allowed to bind the entropy maximization?’ and ‘What if information on amount of data is also available?’. Vagueness of answers to them has given rise in context of linear inverse problems to yet another question: ‘Why MaxEnt?’ This question has been addressed by several axiomatizations (see (Shore and Johnson, 1980), (Tikochinsky, Tishby and Levine, 1984), (Skilling, 1988), (Csiszar, 1991), (Paris and Vencovska, 1997), (Garrett, 1999)) which single out the Shannon’s entropy (or relative entropy) as the only function, consistent with the axioms. Though these axiomatizations answer the most pragmatic ‘Why MaxEnt?’ question, they leave unresolved the first three (‘interpretational’) problems.
3. REM/MaxEnt – as an asymptotic case of MaxProb

Let us consider following general setup.

Let \( q = [q_1, q_2, \ldots, q_m] \) be a pmf, defined on \( m \)-element support, referred to as prior generator.

Let \( \mathcal{H}_n \) be a set of all vectors \( \{n_1, n_2, \ldots, n_J\} \), such that an adding-up constraint \( \sum_{i=1}^{m} n_{ij} = n \), for \( j = 1, 2, \ldots, J \), is satisfied. \( n \) will be referred to as occurrence vector, \( \mathcal{H}_n \) as occurrence-vector working set.

Let \( \mathcal{P} \) be a set of all probability vectors, such that \( \sum_{i=1}^{m} p_i = 1 \).

Then, a simple question can be asked.

**Question 1.** What is the most probable occurrence vector \( \hat{n} \), among occurrence vectors \( n \) from the working set \( \mathcal{H}_n \), to be generated by the prior generator \( q \)?

The answer to the question is

\[
\hat{n} = \arg \max_{n \in \mathcal{H}_n} \pi(n|q) \tag{3.1}
\]

where

\[
\pi(n|q) = \frac{n!}{n_1!n_2! \ldots n_m!} \prod_{i=1}^{m} q_i^{n_i} \tag{3.2}
\]

is the probability of generating the occurrence vector \( n \) by a prior generator \( q \).

**Definition 1.** The above setup and Question 1, leading to task (3.1), (3.2) will be referred to as MaxProb.

The following theorem states the main result on asymptotic equivalence of MaxProb and REM/MaxEnt. The proof is developed in the Appendix A.

**Theorem 1.** Let \( q \) be the prior generator and \( \mathcal{H}_n \) be the working set. Let \( \hat{n} \) be the most probable occurrence vector from the working set \( \mathcal{H}_n \), to be generated by the prior generator \( q \). And let \( n \to \infty \). Then

\[
\frac{\hat{n}}{n} = \hat{p}
\]

where

\[
\hat{p} = \arg \max_{p \in \mathcal{P}} H(p, q)
\]

and

\[
H(p, q) = -\sum_{i=1}^{m} p_i \ln \left( \frac{p_i}{q_i} \right)
\]

is the relative entropy of probability vector \( p \) on generator \( q \).
Corollary. If also some other differentiable constraint $F(n) = 0$ is employed to form the working set $\mathcal{H}_n$, and a corresponding constraint $F(p) = 0$ is added to the relative entropy maximization, the claim of Theorem 1 remains valid.

Note. If the prior generator is uniform, $H(p, q)$ reduces to Shannon’s entropy $H(p) = -\sum_{i=1}^{m} p_i \ln p_i$.

Example. Let $q = [0.13, 0.09, 0.42, 0.36]'$. Let $\mathcal{H}_n$ consists of all occurrence vectors $\{n_1, n_2, \ldots, n_J\}$ such that

$$\sum_{i=1}^{m} n_{ij} = n \quad \text{for} \quad j = 1, 2, \ldots, J$$

$$\sum_{i=1}^{m} n_{ij} x_i = 3.2n \quad \text{for} \quad j = 1, 2, \ldots, J$$

(3.3)

where $x = [1, 2, 3, 4]'$.

Table 1 shows $\hat{p}_n$ and $J$, for $n = 10, 50, 100, 500, 1000$, together with probability vector $\hat{p}$ maximizing relative entropy $H(p, q)$ under constraints

$$\sum_{i=1}^{m} p_i = 1$$

$$\sum_{i=1}^{m} p_i x_i = 3.2$$

(3.4)

Results for uniform prior generator are in the fourth column of the table.

4. Concluding remarks

As a way of summing up we make the following points:

1) The multiplicity argument, as it is left to us by Boltzmann, Wallis, Jaynes, does not provide satisfying rationale for MaxEnt. However it does provide a clue where to search for it.

2) Theorem 1, as any asymptotic theorem, can be interpreted in two directions: either moving towards infinity or moving back to finiteness. The first direction provides the MaxProb rationale for REM/MaxEnt. The second direction shows, that proper place of REM/MaxEnt is only in the asymptotic.
3) MaxProb also automatically solves the known-sample-size problem.

4) Proof of Theorem 1 implies, that constraints that bind REM/MaxEnt should be differentiable.

5) Hidden behind (3.1), (3.2) is an assumption about \textit{iid} sampling. Thus, REM/MaxEnt as an asymptotic form of MaxProb, seem to be limited to the iid case.

The probabilistic rationale for REM/MaxEnt/\(I\)-divergence minimization may also be extended to provide a rationale of \(J\)-divergence minimization, see (Grendar and Grendar, 2000).

Area of applicability of MaxProb/REM/MaxEnt should be obvious – wherever Question 1 is reasonable to ask.

Philosophical consequences of Theorem 1 are left to the reader.

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Appendix

A. Proof of Theorem 1

Proof. 1)

\[
\max_{\mathbf{n}} \pi(\mathbf{n}|\mathbf{q})
\]
subject to

\[
\sum_{i=1}^{m} n_i = n
\]

For the purpose of maximization \( \pi(\mathbf{n}|\mathbf{q}) \) can be log-transformed, into

\[
v(\mathbf{n}) = \gamma(1 + \sum_{i=1}^{m} n_i) - \sum_{i=1}^{m} \gamma(n_i + 1) + l
\]

where \( \gamma(\cdot) = \ln \Gamma(\cdot) \), \( \Gamma(\cdot) \) is gamma-function, and \( l = \sum_{i=1}^{m} n_i \ln q_i \).

Necessary condition for maximum of \( \pi(\mathbf{n}|\mathbf{q}) \) than is

\[
dv(\mathbf{n}) = \sum_{i=1}^{m} \left[ -\gamma'(n_i + 1) + \ln q_i \right] dn_i = 0 \quad (A.1)
\]
since, according to the assumed adding-up constraint, \( \sum_{i=1}^{m} dn_i = 0 \).

First, it will be proved that

\[
\lim_{n_i \to \infty} \left[ \gamma'(n_i) - \ln(n_i + k) \right] = 0 \quad (A.2)
\]

for any \( n_i \), and any \( k \).

The first derivative of \( \gamma \) can be written in a form of infinite series (see (Fichtengoltz, 1969))

\[
\gamma'(n_i) = g(n_i) - C
\]

where

\[
g(n_i) = \sum_{j=0}^{\infty} \left( \frac{1}{j+1} - \frac{1}{j + n_i} \right)
\]

\[C = \text{Euler’s constant}\]
For \( n_i \in \mathbb{Z} \), denoted \( \hat{n}_i \), the series \( g(n_i) \) reduces into a harmonic series \( H \)

\[
g(\hat{n}_i) = \sum_{j=1}^{\hat{n}_i-1} \frac{1}{j} = H(\hat{n}_i - 1)
\]

Let \( n_i = \hat{n}_i + h \), where \( 0 \leq h < 1 \). Then

\[
\frac{1}{j + 1} - \frac{1}{j + \hat{n}_i} \leq \frac{1}{j + 1} - \frac{1}{j + \hat{n}_i + h} < \frac{1}{j + 1} - \frac{1}{j + \hat{n}_i + 1},
\]

so

\[
g(\hat{n}_i) = \sum_{j=1}^{\hat{n}_i-1} \frac{1}{j} \leq g(n_i) < \sum_{j=1}^{\hat{n}_i} \frac{1}{j} = g(\hat{n}_i + 1).
\]

Since, difference of the major series converges to zero,

\[
\lim_{n_i \to \infty} [g(\hat{n}_i + 1) - g(\hat{n}_i)] = \lim_{n_i \to \infty} \frac{1}{n_i} = 0
\]

also

\[
\lim_{n_i \to \infty} [g(n_i) - g(\hat{n}_i)] = 0. \quad \text{(A.3)}
\]

Due to a known property of harmonic series

\[
\lim_{n_i \to \infty} [H(n_i) - \ln(n_i + k) - C] = 0, \text{ for any } k
\]

holds also

\[
\lim_{n_i \to \infty} [g(\hat{n}_i) - \ln(n_i + k) - C] = 0 \quad \text{(A.4)}
\]

thus, adding (A.3), (A.4) up gives

\[
\lim_{n_i \to \infty} [g(n_i) - \ln(n_i + k) - C] = 0,
\]

respectively, for the derivative (recall that \( \gamma'(n_i) = g(n_i) - C \))

\[
\lim_{n_i \to \infty} [\gamma'(n_i) - \ln(n_i + k)] = 0,
\]

what is just (A.2).

Without loss of generality, for \( n \to \infty \) we can restrict for sub-space of \( n_i \to \infty \), for \( i = 1, 2, \ldots, m \), if on the sub-space exists the maximum,
so the conditions of maximum for \( n_i \to \infty \) take, thanks to (A.2), form

\[
\sum_{i=1}^{m} [-\ln n_i + \ln q_i] \, dn_i = 0 \tag{A.5a}
\]

\[
\sum_{i=1}^{m} n_i = n \tag{A.5b}
\]

Due to Lemma 1, with \( k = \frac{1}{n} \), system (A.5) can be transformed into an equivalent one

\[
\sum_{i=1}^{m} \left[ -\ln \frac{n_i}{n} + \ln q_i \right] \, \frac{dn_i}{n} = 0 \tag{A.6a}
\]

\[
\sum_{i=1}^{m} \frac{m}{n} = 1 \tag{A.6b}
\]

2)

\[
\max_{\mathbf{p}} H(\mathbf{p}, \mathbf{q})
\]

subject to

\[
\sum_{i=1}^{m} p_i = 1
\]

Thus necessary conditions for maximum of relative entropy \( H(\mathbf{p}, \mathbf{q}) \), constrained by the respective adding-up constraint are

\[
dH(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^{m} [-\ln p_i + \ln q_i] \, dp_i = 0 \tag{A.7a}
\]

\[
\sum_{i=1}^{m} p_i = 1 \tag{A.7b}
\]

Comparing (A.7) and (A.6) completes the proof. \( \square \)

Note. Claim of the Corollary of Theorem 1 is immediately implied by the proof.

Lemma 1.

\[
dv(k\mathbf{n}) = k \, dv(\mathbf{n})
\]

if \( \sum_{i=1}^{m} n_i = n \).

Proof. \( dv(k\mathbf{n}) = \sum_{i=1}^{m}[-\ln kn_i + \ln q_i] \, dk \, n_i = k \sum_{i=1}^{m}[-\ln k - \ln n_i + \ln q_i] \, dn_i = k \sum_{i=1}^{m}[-\ln n_i + \ln q_i] \, dn_i = k \, dv(\mathbf{n}) \). \( \square \)
B. Expected Occurrence Vector (ExpOc) and REM/MaxEnt

Also, a question different than the Question 1 can be asked.

**Question 2.** What is the expected occurrence vector \( \bar{n} \), of occurrence vectors \( n \) from the working set \( H_n \), which can be generated by the prior generator \( q \)?

Specifying the notion of expectation,

\[
\bar{n} = \frac{\sum_{j=1}^{J} \pi(n_j|q)n_j}{\sum_{j=1}^{J} \pi(n_j|q)}
\]

(B.1)

**Theorem 2.** Let \( q \) be the prior generator and \( H_n \) be the working set. Let \( \bar{n} \) be the expected occurrence vector of the working set \( H_n \), to be generated by the prior generator \( q \). And let \( n \to \infty \). Then, using notation of Theorem 1,

\[
\frac{n}{n} = \hat{p}
\]

**Corollary.** If also a moment consistency constraint is employed to form the working set \( H_n \), and corresponding constraint is added to the relative entropy maximization, the claim of Theorem 2 remains valid.

**Note.** Generality of Corollary 2 is under both numerical and theoretical investigations. Theorem 2 and its Corollary, although yet supported only by numerical calculations, indicates that MaxEnt/REM can be as well an asymptotic form of another method/principle – ExpOc – which concentrates on looking for an expected occurrence vector in the feasible set of vectors generated by a prior generator/pmf.

Following example illustrates the point of Theorem 2/Corollary 2.

**Example.** Assuming the same setup as in the previous Example, expected occurrence vectors for \( n = [10, 50, 100, 1000] \) and generators \( q = [0.13 0.09 0.42 0.36]' \), \( q = [0.25 0.25 0.25 0.25]' \) are in Table 2.

Note that \( \frac{n}{n} \) converges to \( \hat{p} \) faster than \( \frac{\bar{n}}{\bar{n}} \).
Table II. ExpOc and REM/MaxEnt

| n   | \( \frac{\bar{q}}{q} \) | \( \frac{\bar{p}}{p} \) uniform prior |
|-----|----------------|----------------------------------|
| 10  | 0.0721 0.0736 0.4365 0.4178 | 0.0701 0.1510 0.2877 0.4912 |
| 50  | 0.0806 0.0714 0.4153 0.4327 | 0.0771 0.1471 0.2745 0.5013 |
| 100 | 0.0816 0.0712 0.4128 0.4344 | 0.0779 0.1466 0.2729 0.5025 |
| 500 | 0.0824 0.0710 0.4108 0.4358 | 0.0786 0.1463 0.2717 0.5035 |
| 1000| 0.0825 0.0709 0.4106 0.4360 | 0.0787 0.1462 0.2715 0.5036 |
| \( \bar{p} \) | 0.0826 0.0709 0.4103 0.4361 | 0.0788 0.1462 0.2714 0.5037 |

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