

Maximum Entropy method with non-linear moment constraints: challenges

M. Grendar, Jr. and M. Grendar

*Institute of Mathematics and Computer Science of Mathematical Institute of Slovak Academy of Sciences (SAS) and of Matej Bel University, Severná ulica 5, 974 00 Banská Bystrica, Slovakia & Institute of Measurement Science of SAS, Dúbravská cesta 9, 841 04 Bratislava, Slovakia.
umergren@savba.sk*

Abstract. Traditionally, the Method of (Shannon-Kullback's) Relative Entropy Maximization (REM) is considered with linear moment constraints. Here, the method is studied with frequency moment constraints which are non-linear in probabilities. The constraints challenge some justifications of REM: a) Probabilistic justification of REM via Conditioned Weak Law of Large Numbers cannot be invoked since the feasible set of distributions which is defined by frequency moment constraints admits several entropy maximizing distributions (I-projections), b) Axiomatic justifications of REM are developed for linear moment constraints/convex sets. However, REM is not left completely unjustified in this setting, since Entropy Concentration Theorem and Maximum Probability Theorem can be applied.

Maximum Rényi/Tsallis' entropy method (maxTent) is as well considered here due to non-linearity of X-frequency moment constraints which are used in Non-extensive Thermodynamics. It is shown that under X-frequency moment constraints maxTent distribution can be unique and different than the I-projection. This implies that maxTent does not choose the most probable distribution and that the maxTent distribution is asymptotically conditionally improbable. Thus, what are adherents of maxTent accomplishing when they maximize Rényi's or Tsallis' entropy?

1 INTRODUCTION

Let Π be a set of empirical probability mass functions (types) which are defined on m -element support and which can be based on random samples of size n . Let the supposed source of the types be probability mass function \mathbf{q} . A problem (from category of ill-posed inverse problems) of recovering probability distribution from Π amounts to selection of type(s) from Π , in particular when $n \rightarrow \infty$.

The problem (called hereafter Boltzmann-Jaynes Inverse Problem, BJIP, [26], [27], [28]) can be met in many branches of science, ranging from Statistical Physics (where it originated) to Computer Tomography. Several approaches to the problem can be found in the literature. While most of them are tailored to needs of the particular branch of science, the method of (Shannon-Kullback's) Relative Entropy Maximization (REM) is considered as the general solution to the problem by mathematicians. Arguments which justify application of REM for selection of distribution from Π in BJIP range from axiomatic, through probabilistic and game-theoretic to pragmatic, and others. As rule, in order to be valid they put certain requirements on Π and n .

So far, most of the REM-justifying work concentrated on the case of Π defined by the usual linear moment constraints. Such Π possesses the attractive property of con-

vexity, which thanks to concavity of the Shannon-Kullback's entropy implies uniqueness of REM-selected distribution (called I-projection of \mathbf{q} on Π , in the Information Theory). Linearity of the constraints lays behind the well-known exponentiality of the I-projection.

As [38] indicates, so-called frequency moment constraints appear rather naturally in several places in Physics. Frequency moments are non-linear in probabilities and the feasible set Π_f which they define is non-convex. Due to the non-linearity and a symmetry of the constraints, there are multiple I-projections of \mathbf{q} on Π_f . The non-linearity of moments, non-convexity of the feasible set, non-exponentiality of recovered distribution and its non-uniqueness challenge several justifications of REM. Two of the most widely employed REM-justifying arguments: axiomatizations and Conditioned Weak Law of Large Numbers cannot be invoked in this setting since axiomatic systems are developed for linear constraints and CWLLN requires assumption of uniqueness of I-projection. Is there then any reason to select the most entropic distribution from Π_f ? Yes, since Entropy Concentration Theorem (ECT) and Maximum Probability Theorem (MPT) can be readily used to justify MaxEnt also in this case. Though MPT was originally stated with unique I-projection in mind, the Theorem can be instantly extended also to the case of multiple I-projections.

The frequency moment constraints can be viewed as a special case of Tsallis' (cf. [42]) or MNNP (cf. [44], [35]) constraints which are used in 'hot topic' Non-extensive Thermodynamics (NET). The constraints are as well non-linear in probabilities. NET has arisen from Tsallis' prescription to select from set which the constraints define such a distribution which maximizes Tsallis' entropy. Thus, in this area REM was displaced (or generalized, if you wish) by maximization of Tsallis' entropy. Besides axiomatic justifications (which are based on extensions of those of REM) and declared success of maxTent in modeling power-law phenomena (which allegedly REM cannot model), there is however yet no probabilistic justification of the method.

The paper is organized as follows: First, the necessary terminology and notation is set down. Then probabilistic justifications of REM: CWLLN, ECT and MPT are reviewed from perspective of their applicability in the case of multiple I-projections. Maximum Probability Theorem is stated in the general form which covers the situation of multiple I-projections. Also, applicability of other justifications is briefly discussed. Next we turn to the simplest of non-linear moment constraints: frequency moment constraints and note that I-projection on Π_f is non-unique and non-exponential. Frequency moments constraints are then used to provide an illustration for the general form of Maximum Probability Theorem. Next, Tsallis' and Rényi's entropies are introduced, and it is noted that under frequency moment constraints maximization of Rényi-Tsallis' entropy (maxTent) selects no distribution. Under MNNP constraints it does, but as it will be shown, the maxTent-selected distribution can be unique but different than the I-projection. Consequences of this finding for maxTent are discussed. Concluding comments sum up the paper and point to further considerations. Appendix describes a method for finding I-projections on Π_f . Postscript contains a brief reply to Professor Skilling's note.

2 TERMINOLOGY AND NOTATION

Let $\mathcal{X} \triangleq \{x_1, x_2, \dots, x_m\}$ be a discrete finite set called support, with m elements and let $\{X_l, l = 1, 2, \dots, n\}$ be a sequence of size n of identically and independently drawn random variables taking values in \mathcal{X} .

A type $\mathbf{v} \triangleq [n_1, n_2, \dots, n_m]/n$ is an empirical probability mass function which can be based on sequence $\{X_l, l = 1, 2, \dots, n\}$. Thus, n_i denotes number of occurrences of i -th element of \mathcal{X} in the sequence.

Let $\mathcal{P}(\mathcal{X})$ be a set of all probability mass functions (pmf's) on \mathcal{X} . Let $\Pi \subseteq \mathcal{P}(\mathcal{X})$.

Let the supposed source of the sequences (and hence also of types) be $\mathbf{q} \in \mathcal{P}(\mathcal{X})$, called ('prior') generator.

Let $\pi(\mathbf{v})$ denote the probability that \mathbf{q} will generate type \mathbf{v} , i.e., $\pi(\mathbf{v}) = \frac{n!}{n_1! n_2! \dots n_m!} \prod_{i=1}^m q_i^{n_i}$. Then, $\pi(\mathbf{v} \in \mathcal{A})$ denotes the probability that \mathbf{q} will generate a type \mathbf{v} which belongs to $\mathcal{A} \subseteq \Pi$, i.e., $\pi(\mathbf{v} \in \mathcal{A}) = \sum_{\mathbf{v} \in \mathcal{A}} \pi(\mathbf{v})$. Finally, let $\pi(\mathbf{v} \in \mathcal{A} | \mathbf{v} \in \Pi)$ denote the conditional probability that if \mathbf{q} generates type $\mathbf{v} \in \Pi$ then the type belongs to \mathcal{A} . It is assumed that the conditional probability exists.

I-projection $\hat{\mathbf{p}}$ of \mathbf{q} on set $\Pi \subseteq \mathcal{P}(\mathcal{X})$ is such $\hat{\mathbf{p}} \in \Pi$ that $I(\hat{\mathbf{p}} \| \mathbf{q}) = \inf_{\mathbf{p} \in \Pi} I(\mathbf{p} \| \mathbf{q})$, where¹ $I(\mathbf{p} \| \mathbf{q}) \triangleq \sum_{\mathcal{X}} p_i \log \frac{p_i}{q_i}$ is the I-divergence. I-divergence is known under various other names: Kullback-Leibler's distance, KL number, Kullback's directed divergence, etc. When taken with minus sign it is known as (Shannon-Kullback's) relative entropy.

General framework of this work is established by Boltzmann-Jaynes inverse problem (BJIP)²:

Let there be a set $\Pi \subseteq \mathcal{P}(\mathcal{X})$ of types which are defined on m -element support \mathcal{X} and which can be based on random samples of size n . Let the supposed source of the random samples (and thus also types) be \mathbf{q} . BJIP amounts to selection of specific type(s) from Π when information $\{\mathcal{X}, n, \mathbf{q}, \Pi\}$ is supplied.

Example 1: Let $n = 6$, $\mathcal{X} = [1 \ 2 \ 3]$, $\mathbf{q} = [1/3 \ 1/3 \ 1/3]$ and let the feasible set comprise all such types which have probability of one of the support-points equal to $2/3$, ie. $\Pi = \{[2/3 \ 1/6 \ 1/6], [2/3 \ 1/3 \ 0], \dots\}$ where the dots stand for the remaining 7 permutations of the two listed types. Given the information $\{n, \mathcal{X}, \mathbf{q}, \Pi\}$ the BJIP task is to select a type from the set Π . \diamond

If Π contains more than one type (as it is the case in the above Example), the BJIP becomes under-determined and in this sense ill-posed.

¹ There, $\log 0 = -\infty$, $\log \frac{b}{0} = +\infty$, $0 \cdot (\pm\infty) = 0$, conventions are assumed. Throughout the paper \log denotes the natural logarithm.

² Equivalently the framework could be phrased as a problem of induction (or updating), cf. [21].

3 JUSTIFICATIONS OF REM

3.1 Conditioned Weak Law of Large Numbers

A result of the Method of Types, which was developed in the Information Theory (cf. [11]), provides a probabilistic justification for application of REM method for solving BJIP, when n tends to infinity and Π has certain properties. The result is usually known as Conditioned Weak Law of Large Numbers (CWLLN), or as Gibbs conditioning principle (in large deviations literature, see [14], [12]). The argument shows (loosely speaking) that any type from Π which is generated by \mathbf{q} and is not close (in L_1 -norm) to the I-projection of \mathbf{q} on Π becomes conditionally improbable to come from \mathbf{q} as sample size grows large. To establish this result (cf. [50], [49], [22], [9], [7], [31], [32], [33]) assumption of uniqueness of I-projection is needed.

(CWLLN) *Let $\hat{\mathbf{p}}$ be unique I-projection of \mathbf{q} on closed set Π . Let $\mathbf{q} \notin \Pi$. Then for any $\epsilon > 0$*

$$\lim_{n \rightarrow \infty} \pi(|\mathbf{v}_i - \hat{\mathbf{p}}_i| > \epsilon \mid \mathbf{v} \in \Pi) = 0 \quad i = 1, 2, \dots, m \quad (1)$$

Well-studied is the case of closed, convex Π , which ensures uniqueness of I-projection, provided that it exists (cf. [9], and [31], [32], [33], [23] for further developments). As it is well-known, in this case the I-projection belongs to the exponential family of distributions (see [8]).

3.2 Entropy Concentration Theorem

Without the assumption of uniqueness of the I-projection, a claim known as the Entropy Concentration Theorem (ECT), weaker than (1), can be still made (see [7]):

(ECT) *Let $\Pi \subseteq \mathcal{P}(\mathcal{X})$ be nonempty closed set. Let $\hat{\mathbf{I}}$ be such that $\hat{\mathbf{I}} \leq \mathbf{I}(\mathbf{v} \parallel \mathbf{q})$ for any $\mathbf{v} \in \Pi$. Then for any $\epsilon > 0$*

$$\lim_{n \rightarrow \infty} \pi(|\mathbf{I}(\mathbf{v} \parallel \mathbf{q}) - \hat{\mathbf{I}}| < \epsilon \mid \mathbf{v} \in \Pi) = 1 \quad (2)$$

Assumption (of whatever form) which guarantees existence and uniqueness of the I-projection is crucial for coming from statement (2) to the stronger claim (1).

3.3 Maximum Probability Theorem

Maximum Probability Theorem (MPT), which was originally (see [16], Thm 1) stated with unique I-projection in mind, claims that the type $\hat{\mathbf{v}}$ in Π which the ('prior') generator \mathbf{q} can generate with the highest probability converges to the I-projection of \mathbf{q} on Π , as $n \rightarrow \infty$. However proof of the Theorem (cf. [16]) covers more general situation of multiple I-projections and thus allows to state MPT in the following general form:

(MPT) Let \mathbf{q} be a generator. Let differentiable constraint $F(\mathbf{v}) = 0$ define feasible set of types $\Pi_n \subseteq \Pi$ and let $\Pi \triangleq \{\mathbf{p} : F(\mathbf{p}) = 0\}$ be the corresponding feasible set of probability mass functions. Let $\hat{\mathbf{v}}_j \triangleq \arg \max_{\mathbf{v} \in \Pi_n} \pi(\mathbf{v})$, $j = 1, 2, \dots, l$, be types which have among all types from Π_n the highest probability of coming from the generator \mathbf{q} . Let there be k I-projections $\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2, \dots, \hat{\mathbf{p}}_k$ of \mathbf{q} on Π . And let $n \rightarrow \infty$. Then $l = k$ and $\hat{\mathbf{v}}_j = \hat{\mathbf{p}}_j$, for $j = 1, 2, \dots, k$.

It should be noted that MPT argument implies that REM is only a special, asymptotic form of simple and self-evident method (called Maximum Probability method (Max-Prob) at [16]) which seeks in Π such types which the generator \mathbf{q} can generate with the highest probability. Thus applicability of REM in BJIP is inherently limited to the case of sufficiently large n .

From the perspective of the current work, it is important that the MPT holds also when the feasible set admits multiple types with the highest value of the probability π . An illustration of the convergence of most probable types to I-projections will be given in the Section 4, where such a set is determined by frequency moment constraints.

3.4 Axiomatic systems

Besides the probabilistic arguments several axiomatic approaches were developed to support maximization of Shannon's entropy or relative entropy as the only logically consistent method for solving BJIP³. However, it should be noted that maximization of Rényi's entropy was as well found to satisfy some of the axiomatic systems, which had been developed to justify REM (see [47]). For purposes of the presented work it is sufficient to note that the axiomatic system (cf. [10]) which is perhaps the most widely accepted requires assumption of linearity of the constraints (or, in general, convexity of Π and hence, uniqueness of I-projection). A non-axiomatic argument based on potential-probability density relationship and a complementarity (cf. [18]) is restricted to the linear constraints as well. Also a game-theoretic view of REM (see [24]) assumes the linear constraints.

To sum up: When the set Π admits several I-projections the justifications of REM which are readily available reduce to Entropy Concentration Theorem and Maximum Probability Theorem. At the next section, such set will be defined by means of frequency moment constraint⁴.

4 FREQUENCY MOMENT CONSTRAINTS

This study was triggered by an interesting paper by Romera, Angulo and Dehesa (cf. [38]) on frequency moment problem. There also links to statistical considerations of the

³ Strictly speaking, the axiomatizations assume BJIP with either n unknown or n bigger than any limit. They seem to be inappropriate for BJIP with finite sample size.

⁴ Note, however, that Π which admits multiple I-projections can be defined also by means of the usual linear moments (cf. [20]).

frequency moments as well as to their applications in Physics can be found.

In the simplest case of single frequency moment constraint, feasible set of types is defined as $\Pi_f \triangleq \{\mathbf{p} : \sum_{i=1}^m p_i^\alpha - \alpha = 0, \sum_{i=1}^m p_i - 1 = 0\}$, where $\alpha, \alpha \in \mathbf{R}$. If $m > 2$, the problem of selection of type becomes ill-posed. Note that the first constraint is for $\alpha \neq 1$ non-linear in \mathbf{p} and Π_f is non-convex.

4.1 I-projection: non-uniqueness and non-exponentiality

It is straightforward to observe that I-projection of \mathbf{q} on Π_f possesses a symmetry, in the sense that if certain $\hat{\mathbf{p}}$ is I-projection of \mathbf{q} on Π_f then any permutation of the vector $\hat{\mathbf{p}}$ should necessarily be also I-projection.

Within this Section \mathbf{q} will be assumed uniform (for a reason which is implied by discussion at Section 5.1), denoted \mathbf{u} . Note that when uniform generator is assumed, the method of Relative Entropy Maximization reduces to Maximum Shannon's Entropy method (abbreviated usually MaxEnt).

The non-convexity of feasible set makes the problem of maximization of Shannon's entropy analytically unsolvable. Critical value of p_i is expressed as: $p_i(\lambda) = k(\lambda)e^{-\lambda\alpha p_i^{\alpha-1}}$, where $k(\lambda) = \sum e^{-\lambda\alpha p_i^{\alpha-1}}$. Note that the expression is explicitly self-referential.

Thus, the I-projections should be searched out either numerically or by a method which is described at the Appendix.

4.2 MaxProb justification of REM: multiple I-projections

That the most probable types indeed converge to the corresponding I-projections as the general form Maximum Probability Theorem states will be illustrated by the following Example.

Example 2: Let $\alpha = 2$, $\mathcal{X} = [1\ 2\ 3]$, $m = 3$ and $\alpha = 0.42$ (the value was obtained for $\mathbf{p} = [0.5\ 0.4\ 0.1]$).

For $n = 10, 30, 330, 1000, 2000$ the feasible sets Π_f were constructed. For example, $\Pi_{f,10}$ contains $\mathbf{v} = [5\ 4\ 1]/10$ and all its permutations (ie. $[5\ 1\ 4]/10$, etc). This will be called *group of types*. $\Pi_{f,30}$ contains two groups: $[15\ 12\ 3]/30$ and $[17\ 8\ 5]/30$. The last one has higher probability of coming from uniform prior generator. For $n = 330$ the feasible set comprises groups $[0.0939\ 0.4333\ 0.4727]$, $[0.5666\ 0.2666\ 0.1666]$, $[0.1\ 0.4\ 0.5]$ and the group $[0.1939\ 0.2333\ 0.5727]$, which has the highest probability of being generated by \mathbf{u} .

For each n , among the feasible types, the most probable $\hat{\mathbf{v}}$ which could be drawn from the uniform prior generator was picked up. They are stated at the Table 1 together with a corresponding I-projection of \mathbf{u} on Π_f .

Clearly, the most probable type (hence also the whole permutation group of 6 most probable types) converges to the pmf (permutation group of 3 pmf's) which maximizes Shannon's entropy. \diamond

TABLE 1. The most probable type, for growing n .

n	$\hat{\mathbf{v}} \mathbf{u}$		
10	0.1	0.4	0.5
30	0.166	0.266	0.566
330	0.1939	0.2333	0.5727
1000	0.1990	0.2280	0.5730
2000	0.2080	0.2185	0.5735
$\hat{\mathbf{p}}$	0.2131	0.2131	0.5737

4.3 maxTent: no selection

At this point, both Rényi's and Tsallis' entropies will be introduced. Rényi's entropy (cf. [39], [37]) is defined as $H_R(\mathbf{p}) \triangleq \frac{1}{1-\alpha} \log(\sum_{i=1}^m p_i^\alpha)$, where $\alpha \in \mathbf{R}$, $\alpha \neq 1$.

Tsallis' entropy H_T (cf. [25], [48], [42]) is linear approximation of Rényi's entropy: $H_T(\mathbf{p}) \triangleq \frac{1-\sum_{i=1}^m p_i^\alpha}{\alpha-1}$, where $\alpha \in \mathbf{R}$, $\alpha \neq 1$.

Rényi's entropy attains its maximum at the same pmf as does Tsallis' entropy. Thus, hereafter maxTent will denote both method of maximum Rényi's and Tsallis' entropy at once. maxTent will be discussed in greater detail in Section 5. Here it suffices to note that in the set Π_f which is defined by the frequency moment constraint each type has the same value of Rényi's (or Tsallis') entropy. In other words, maxTent refuses to make a choice from Π_f . Recall that MaxEnt selects the I-projections, and ECT implies that types conditionally concentrate on the I-projections in such a way, that as n gets large there is virtually no chance to find a type which has value of Shannon's entropy different than the maximal one. MPT complements it by stating that most probable types turn into the I-projections, as n goes to infinity.

5 X-FREQUENCY MOMENT CONSTRAINTS

Frequency moment constraints can be viewed as a special case of non-linear constraints which were originally introduced into Statistical Mechanics by Tsallis (see [42]). Tsallis' constraints define feasible set $\Pi_T \triangleq \{\mathbf{p} : \sum_{i=1}^m p_i^\alpha x_i - \alpha = 0, \sum_{i=1}^m p_i - 1 = 0\}$.

Tsallis' constraints were for Physics reasons superseded by TMP constraints (see [44]). Later on, the TMP constraints were rearranged by Martínez, Nicolás, Pennini and Plastino [35] in MNPP form which allows for simpler analytic tractability. The TMP constraints in MNPP form specify feasible set as $\Pi_\tau \triangleq \{\mathbf{p} : \sum_{i=1}^m p_i^\alpha (x_i - b) = 0, \sum_{i=1}^m p_i - 1 = 0\}$. A probability mass function (pmf) from Π_τ at which Tsallis' (or Rényi's) entropy attains its maximum will be called τ -projection.

Since an argument which is presented at Section 5.4 is valid both for Tsallis' constraints and MNPP constraints, both they will be referred hereafter as X-frequency moment constraints.

5.1 maxTent: backward compatibility with MaxEnt

Non-extensive Thermodynamics (NET) prescribes to use maximization of Tsallis' entropy for the pmf selection when the feasible set is defined by X -frequency constraints. As it was already mentioned, the distribution selected by maximization of Tsallis' entropy is the same as that by Rényi's entropy maximization. Though it is not our concern here, for completeness it should be noted that Rényi's entropy is extensive (additive) whilst Tsallis' one is not, and that the 'world according to Rényi' has different properties than the 'world according to Tsallis' (see [29]).

Maximization of Rényi-Tsallis' entropy under X -frequency constraints satisfies the elementary requirement of backward compatibility with MaxEnt: when X -frequency constraints reduce to the classic linear moment constraints, the Tsallis' entropy reduces to Shannon's one (it happens for $\alpha \rightarrow 1$). In relation to this, it should be noted that maximization of Shannon's entropy is from the point of view of probabilistic justifications just a special case (uniform \mathbf{q}) of Relative Entropy Maximization. However no relative form of Tsallis' entropy was yet considered by adherents of NET. For this reason in our considerations general prior distribution \mathbf{q} is replaced by uniform one, \mathbf{u} .

5.2 MaxEnt: non-exponentiality maxTent: power law

Maximization of Shannon's entropy under MNNP form of X -frequency moment constraints by Lagrange multiplier technique leads to pmf which is of implicit and self-referential form, only: $p_i(\lambda) \propto e^{-\lambda\alpha(x_i-b)p_i^{\alpha-1}}$. Whether it is the I-projection and whether it is unique cannot be analytically assessed.

Under MNNP constraints, maximization of Rényi-Tsallis' entropy by means of Lagrangean leads to the first order conditions for extremum which are solved by a pmf of power-law form: $p_i(\lambda) \propto (1 + \lambda x_i(\alpha - 1))^{1/(1-\alpha)}$ (see [35]). It is important to note, that the candidate pmf could be a (local/global) maximum only if $\alpha > 0$ and if $1 + \lambda x_i(\alpha - 1) > 0$ for all $i = 1, 2, \dots, m$. The latter requirement, known as Tsallis' cut-off condition, should be checked on the case-by-case basis.

5.3 Generalized entropies and BJIP

Non-shannonian forms of entropies have been around for long time. Some of them fall into category of convex statistical distances, and their mathematical properties are well-studied (cf. [34]). Also, extensions and modifications of axiomatic systems which lead to non-shannonian entropies were studied (see [3]). Some of the 'new' entropies were found useful, some not (cf. [2]). As far as Rényi's entropy is concerned few its 'operational characterizations' were developed in the Information Theory (cf. [1] and literature cited therein). Little seems to be known however about its probabilistic justification in context of the ill-posed inverse problems. In particular, it is not known what is the probabilistic question that maxTent answers. Neither it is known, whether

the unknown question which maxTent answers is meaningful to ask within the context of BJIP.

5.4 MaxEnt vs. maxTent

maxTent method is by adherents of NET presented as a generalization of MaxEnt. The generalization extends MaxEnt in two directions: Shannon's entropy is generalized into the Tsallis' entropy, and the traditional linear moment constraints are generalized into non-linear either Tsallis' constraints or MNNP constraints. Though there can be no objection made to generalization of constraints, rather vague arguments (see for instance Introduction of [45]) were advanced to explain why maximization of Shannon's entropy should be under the X-frequency constraints replaced by maximization of Tsallis' entropy to select a distribution from the feasible set which the constraints define.

Conditioned Weak Law of Large Numbers (or Gibbs conditioning principle), Entropy Concentration Theorem and Maximum Probability Theorem provide probabilistic justification of REM (and hence also of MaxEnt) method (though adherents of maxTent might failed to note it, see [46]). As it was discussed here, ECT and MPT can be readily used also under any non-linear constraints, and hence the two Theorems give justification to application of REM/MaxEnt also under Tsallis' or MNNP constraints. Thus, when n is sufficiently large (which is indeed the case in Statistical Mechanics), anybody who chooses from the feasible set which is defined by say MNNP constraints the I-projection(s) can be sure 1) that (any of) the I-projection is just such a type in the feasible set which can be drawn from \mathbf{q} with the highest probability when n goes to infinity (recall MPT), and moreover that 2) any type which has not value of the relative entropy close to the maximal value which is attainable within the feasible set is asymptotically conditionally improbable (recall ECT).

In an interesting paper [30] which for the first time exposed maxTent to a criticism from a probabilistic point of view, La Cour and Schieve derived necessary conditions for agreement of I- and τ -projections under MNNP constraints. Also, the authors illustrated by means of specific example ($\alpha = 1/2$, $m = 3$, $\mathbf{X} = [1 \ 2 \ 3]$ and $\alpha = 7/11$) that τ -projection can be different than I-projection. Provided that the I-projection is unique, one can safely recall CWLLN to conclude that maxTent-selected τ -projection on Π_τ is asymptotically conditionally improbable. However, the issue of uniqueness or non-uniqueness of I-projection on Π_τ is to the best of our knowledge not settled yet.

A different argument is used here to show that maxTent can select asymptotically conditionally improbable distribution under X-frequency constraints. The argument is based on observation that by a choice of support points of the random variable \mathbf{X} the feasible set of distributions Π_τ can be made convex (the same can be done with Π_τ). Convexity of Π_τ guarantees uniqueness of I-projection. Provided that $\alpha > 0$ (which implies concavity of Tsallis' entropy) the τ -projection on the convex Π_τ is as well unique. Both I-projection and τ -projection can be then found out by straightforward analytic maximization. Since the two are (except of trivial cases) different, CWLLN implies that the one chosen by maxTent has asymptotically zero conditional probability.

The next Example illustrates the argument.

Example 3: Let $\Pi_\tau = \{\mathbf{p} : \sum_{i=1}^3 p_i^2(x_i - b) = 0, \sum_{i=1}^3 p_i - 1 = 0\}$. Let $\mathcal{X} = [-2 \ 0 \ 1]$ and let $b = 0$. Then $\Pi_\tau = \{\mathbf{p} : p_3^2 = 2p_1^2, \sum p_i - 1 = 0\}$ which effectively reduces to $\Pi_\tau = \{\mathbf{p} : p_2 = 1 - p_1(1 + \sqrt{2}), p_3 = \sqrt{2}p_1\}$. Prior generator \mathbf{q} is assumed to be uniform \mathbf{u} .

The feasible set Π_τ is convex. Thus I-projection $\hat{\mathbf{p}}$ of \mathbf{u} on Π_τ is unique, and can be found by direct analytic maximization to be $\hat{\mathbf{p}} = [0.2748 \ 0.3366 \ 0.3886]$. Straightforward maximization of Rényi-Tsallis' entropy lead to unique τ -projection $\hat{\mathbf{p}}_\tau = [0.2735 \ 0.3398 \ 0.3867]$, which is different than $\hat{\mathbf{p}}$. \diamond

The finding that τ -projection can be asymptotically conditionally improbable prompts Jaynes question: What are adherents of maxTent accomplishing when they maximize Rényi-Tsallis' entropy?

6 CONCLUDING COMMENTS

Frequency moment constraints, which are the simplest of non-linear constraints, were employed in this work to define feasible set of types Π_f for Boltzmann-Jaynes Inverse Problem. Non-linearity of the frequency constraints implies non-convexity of the feasible set, and together with their symmetry also non-uniqueness of I-projection. Moreover, because of the non-linearity, I-projections of \mathbf{q} on the feasible set Π_f do not take the canonical exponential form⁵.

The non-linearity, and implied non-convexity, non-uniqueness and non-exponentiality revealed limitations of several justifications of the REM/MaxEnt method. However, REM is not left completely unjustified in this non-traditional setup, since two justifications of REM are provided by Entropy Concentration Theorem and Maximum Probability Theorem. Thus though REM under frequency constraints loses two of its charming properties: uniqueness and exponentiality of I-projection, its application within the corresponding BJIP remains justified by the two Theorems.

One of the primary aims of this work was to give a general (multiple I-projection) formulation of Maximum Probability Theorem and provide its illustration. At the same time the work was intended to serve as an invitation to considerations of non-convex sets and non-unique I-projections which challenge several traditional justifications of REM/MaxEnt⁶. Though here such sets were constructed by means of non-linear moment constraints, it should be noted that non-convex sets with multiple I-projections can be defined as well by linear moment constraints (see [20]).

⁵ It obviously does not mean that they cannot be ex post brought into the canonical exponential form. Any vector of non-negative numbers which add up to one is MaxEnt canonical distribution, recall [5], Thm. 4.1.

⁶ In particular, they call for reconsideration of CWLLN. The law states that types conditionally concentrate on the I-projection, provided that the last is unique. What if Π admits several I-projections? Do types concentrate on each of the I-projections? If yes, what is the proportion? Answers to these questions were given elsewhere (see [20]). In order to leave the reader chance to appreciate extent of the challenges which multiple I-projections pose to justifications of REM/MaxEnt the present paper was intentionally written as if the answers to these questions were not known.

Maximum Rényi/Tsallis' entropy method (maxTent) was considered here mainly because of the non-linearity of the constraints which are used in Non-extensive Thermodynamics (NET). As it was shown (see Sect. 5), under the constraints maxTent can select a distribution which is according to CWLLN asymptotically conditionally improbable. This finding prompts Jaynes question: What are adherents of maxTent accomplishing when they maximize Rényi-Tsallis' entropy? When it will be answered, maxTent could enter the tiny class of entropies for which the answer is known and which can thus be consciously applied for distribution selection.

ACKNOWLEDGEMENTS

Hospitality of Banach Centre (BC) of the Institute of Mathematics of Polish Academy of Sciences, where a part of this study was performed as a part of the European Community Center of Excellence programme (package 'Information Theory and its Applications to Physics, Finance and Biology') is gratefully acknowledged. The work was also supported by the grant VEGA 1/0264/03 from the Scientific Grant Agency of the Slovak Republic. MG Jr gratefully acknowledges financial support of his participation at MaxEnt 23 from E. T. Jaynes International Center.

It is a pleasure to thank Brian R. La Cour for very valuable discussions and comments on [19]. The thanks extend also to Aleš Gottvald, George Judge, John Skilling, Jonathan D. H. Smith, Alberto Solana-Ortega, Myron Tribus and Viktor Witkowský.

APPENDIX

Observe, that any of the three I-projections at the Example 2 (Section 4.2) has two of probabilities equal. This can be elucidated by the following elementary considerations: suppose that the feasible set is constrained further by additional requirement $p_1 = p_2 = p_3$. This additional requirement makes $\mathbf{p}_0 = [1/3 \ 1/3 \ 1/3]$ the only pmf in the set. Clearly, the pmf is indeed in the set only if $\alpha \equiv \alpha_0 = 1/3$, ie. the 'centre of mass' of $\sum_{i=1}^3 p_i^2$. If $\alpha \neq \alpha_0$ then \mathbf{p}_0 is not in Π_f , hence the most entropic pmf should be searched among those pmf's which have two of probabilities equal; say $p_1 = p_2$.

The additional requirement turns the under-determined conditions into a quadratic equation which is solved by either $p_1 = 0.2131$ or $p_1 = 0.4535$. Hence the restricted feasible set comprises two groups of pmf's $[0.2131 \ 0.2131 \ 0.5737]$ and $[0.4535 \ 0.4535 \ 0.0930]$. The first pmf has Shannon's entropy $H_U = 0.9777$, the second $H_L = 0.9381$. It does not surprise that pmf's from the original set Π_f (ie. those which can have all three probabilities different) have Shannon's entropy within the bounds which are set up by H_L and H_U .

This is obviously, not a property specific to the studied example with the particular choice of $\alpha = 2$ and $m = 3$. In general, the finding permits to state the following

Proposition *Let \mathbf{q} be uniform, $\Pi_f \triangleq \{\mathbf{p} : \sum p_i^\alpha - \alpha = 0, \sum p_i - 1 = 0\}$, where $\mathbf{p} \in \mathbf{R}^m$ and $\alpha \in \mathbf{Z}$. Let $m > \alpha$. Then $\hat{\mathbf{p}} \in \Pi_f$ such that $H(\mathbf{p}) \leq H(\hat{\mathbf{p}})$ for any $\mathbf{p} \in \Pi_f$, is such that*

$\hat{p}_1 = \hat{p}_2 = \dots = \hat{p}_{m-1}$, where \hat{p}_1 is one of solutions of the following algebraic equation:

$$(m-1)\hat{p}_1^\alpha + (1 - (m-1)\hat{p}_1)^\alpha - \alpha = 0 \quad (3)$$

Note: Clearly, among the pmf's which solve equation (3), $\hat{\mathbf{p}}$ is the one with the highest value of Shannon's entropy H . Any permutation of $\hat{\mathbf{p}}$ is also I-projection of \mathbf{u} on Π_f .

POSTSCRIPT

At [40] a fundamental question, whether probabilities could be used non-linearly in the integral/expectation, especially if they are viewed as a measure, was risen. Let (Ω, S, P) be the usual probability space, $X : \Omega \rightarrow \mathbb{R}$ a measurable function and μ the induced measure/law dominated by a measure λ . The Lebesgue integral $\int X d\mu$ can be constructed in the standard way and expressed in terms of the Radon-Nikodym derivative f as $\int X f d\lambda$. Afterwards an α -integral: $\int X f^\alpha d\lambda$, $\alpha \in \mathbb{R}$, can be defined as a meaningful object which (in our view) does not contradict the measure/probability theory.

BIBLIOGRAPHIC NOTE

Literature on Tsallis' maximum entropy method is vast (cf. [43]). arXiv contains a series of preprints which document evolution of the method. Also, see March 2002 issue of Chaos, Solitons and Fractals, see also [6]. Critical voices are rare (cf. [30], [15], [51], [41]). This work draws on and corrects [19].

REFERENCES

1. Arikan E., *IEEE Trans. IT*, **42**, No 1, 99-105, (1996).
2. Aczél, J., *Aequa. Math.*, **27**, 1-19, (1984).
3. Aczél, J., and Daróczy, Z., *On Measures of Information and Their Characterizations*, Academic Press, New York, (1975).
4. Anteneodo, C. and Plastino, A. R., *J. Phys. A* **32**, 1089, 1999.
5. Athreya, K. B. and Smith, J. D. H., *Disc. Math. Prob. Stat.*, **20**, 167-176, (2000).
6. Cohen, E. G. D., "Some recent advances in classical statistical mechanics," in LNP 597, P. Garbaczewski and R. Olkiewicz (eds.), pp. 7-33, Springer-Verlag, Berlin, (2002).
7. Cover, T. and Thomas, J., *Elements of Information Theory*, Wiley, 1991.
8. Csiszár, I., *Ann. Prob.*, **3**, No. 1, 146-158, (1975).
9. Csiszár, I., *Ann. Prob.*, **12**, No. 3, 768-793, (1984).
10. Csiszár, I., *Ann. Stat.*, **19**, 2032 - 2066, (1991).
11. Csiszár, I., *IEEE Trans. IT*, **44**, No. 6, 2505-2523, (1998).
12. Dembo, A and Zeitouni, O., *Large Deviations Techniques and Applications*, 2-nd ed., Springer, Application of Mathematics, vol. 38, 1998.
13. Ellis, R. S., *Physica D*, 106-136, (1999).
14. Ellis, R. S., *Entropy, Large Deviations and Statistical Mechanics*, Springer-Verlag, NY, 1985.
15. Gottvald, A., "Beyond the MaxEnt Principle: Bayes, Fourier, Zipf and Spirals in Metamorphoses," *Energy and Information in Non-linear Systems*, A. Gottvald (ed.), pp. 48-51, 2000.

16. Grendár, M., Jr. and Grendár, M., "What is the question that MaxEnt answers? A probabilistic interpretation," in *Bayesian inference and Maximum Entropy methods*, A. Mohammad-Djafari (ed.), pp. 83-94, AIP, 2001. Also uk.arxiv.org/pdf/math-ph/0009020, Sep 2000.
17. Grendár, M., Jr. and Grendár, M., *Entropy*, **3**, 58-63, (2001).
18. Grendár, M., and Grendár, M., Jr., "Why Maximum Entropy? A non-axiomatich approach," in *Bayesian inference and Maximum Entropy methods*, R. L. Fry (ed.), pp. 375-379, AIP, 2002. Also at uk.arxiv.org/pdf/math-ph/0212005, Dec 2002.
19. Grendár, M., Jr. and Grendár, M., "Frequency moments inverse problem and Maximum (Shannon vs Renyi-Tsallis) Entropy. A case study in MaxProb," IMPAN preprint, 2002.
20. Grendár, M., Jr. and Grendár, M., *Acta U. Belii Ser. Math.*, **10**, 3-8, (2003).
21. Grendár, M., Jr. and Grendár, M., "Maximum Probability and Maximum Entropy methods: bayesian interpretation," this proceedings.
22. Grooneboom, P., Oosterhoff, J. and Ruymgaart, F. H., *Ann. Prob.*, **7**, 553-586, (1979).
23. Harremoës, P., "Information topologies with applications," to appear at *Bolyai Studies*.
24. Harremoës, P. and Topsøe, F., *Entropy*, **3**, 191-226, (2001).
25. Havrda, J. and Charvát, F. *Kybernetika*, **3**, 30-35, (1967).
26. Jaynes, E. T., *Papers on Probability, Statistics and Statistical Physics*, R. D. Rosenkrantz (ed.), D. Reidel, Dordrecht, 1979.
27. Jaynes, E. T., "Prior information and ambiguity in inverse problems," in *Inverse Problems*, D. W. McLaughlin (ed.), p. 151, Am. Math. Soc., Providence, RI, [SIAM-AMS Proceedings **14**], 1984.
28. Jaynes, E. T., *Probability Theory: The Logic of Science*, G. Larry Bretthorst (ed.), CUP, NY, 2003.
29. Jizba, P. and Arimitsu, T., "The world according to Rényi: thermodynamics of fractal systems," arxiv.org/abs/condmat/0108184, Aug 2001.
30. La Cour, B. and Schieve, W. C., *Phys. Rev. E*, **62**, 7494-7496, (2000). Also, uk.arxiv.org/pdf/condmat/0009216, Sep 2000.
31. La Cour, B. R. and Schieve, W. C., *Jour. Stat. Phys.*, **107**, 3/4, 729-755, (2002).
32. Leonard, Ch. and Najim, J., *Bernoulli*, **8**, 6, 721-743, (2002).
33. Lewis, J. T., Pfister, C.-E. and Sullivan, W. G., *Markov Proc. Rel. Field.*, **1**, pp. 319-386, (1995).
34. Liese, F. and Vajda, I., *Convex Statistical Distances*, BSB B.G. Teubner Verlagsgesellschaft, Teubner - Texte zur Mathematik, Band 95, Leipzig 1987.
35. Martínez, S., Nicolás, F., Pennini, F. and Plastino, A., "Tsallis' entropy maximization procedure revisited," arxiv.org/abs/physics/0003098, Dec 2000.
36. Rajagopal, A. K. and Abe, S., *Chaos, Solitons and Fractals*, **13**, 529-537, (2002).
37. Rényi, A., "On measures of entropy and information," *Proc. 4th Berk. Symp. Math. Statist. and Probl.*, University of California Press, Vol. 1, pp. 547-461, 1961.
38. Romera, E., Angulo, J. C. and Dehesa, J. S., "Reconstruction of a density from its entropic moments," *Bayesian Inference and Maximum Entropy Methods*, R. L. Fry (ed.), pp. 449-457, AIP, 2002.
39. Schützenberger, M. P., "Contribution aux applications statistique de la théorie de l'information," Publ. Inst. Stat, U. Paris, 1954.
40. Skilling, J., personal communication, MaxEnt 23, 2003.
41. Tribus, M., The First E. T. Jaynes Lecture, this proceedings.
42. Tsallis, C., *J. Stat. Phys.*, **52**, 479, (1988).
43. Visit <http://tsallis.cat.cbpf.br/biblio.htm> for a bibliography on maxTent.
44. Tsallis, C., Mendes, R. S. and Plastino, A. R., *Physica A*, **261**, 534-554, (1998).
45. Tsallis, C., "Entropic nonextensivity: a possible measure of complexity," available at uk.arxiv.org/pdf/cond-mat/0010150, Oct 2000.
46. Tsallis, C. and Brigatti, E., "Nonextensive statistical mechanics: a brief introduction," available at arxiv.org/abs/cond-mat/0305606, May 2003.
47. Uffink, J., *Studies Hist. Phil. Modern Phys.*, **26B**, 223-261, (1995).
48. Vajda, I., *Theory of Statistical Inference and Information*, Dordrecht-Boston, KAP, 1989.
49. van Campenhout, J. M. and Cover, T. M., *IEEE IT*, **27**, 483-489, (1981).
50. Vasicek, O. A., *Ann. Prob.*, **8**, 142-147, (1980).
51. Velázquez, L. and Guzmán, F., "Where the Tsallis statistic is valid?," available at uk.arxiv.org/pdf/condmat/0105378, May 2001.

July 2002, May-July 2003