On Tsallis Entropy Bias and Generalized Maximum Entropy Models

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Abstract In density estimation task, maximum entropy model (Maxent) can effectively use reliable prior information via certain constraints, i.e., linear constraints without empirical parameters. However, reliable prior information is often insufficient, and the selection of uncertain constraints becomes necessary but poses considerable implementation complexity. Improper setting of uncertain constraints can result in overfitting or underfitting. To solve this problem, a generalization of Maxent, under Tsallis entropy framework, is proposed. The proposed method introduces a convex quadratic constraint for the correction of (expected) Tsallis entropy bias (TEB). Specifically, we demonstrate that the expected Tsallis entropy of sampling distributions is smaller than the Tsallis entropy of the underlying real distribution. This expected entropy reduction is exactly the (expected) TEB, which can be expressed by a closed-form formula and act as a consistent and unbiased correction. TEB indicates that the entropy of a specific sampling distribution should be increased accordingly. This entails a quantitative re-interpretation of the Maxent principle. By compensating TEB and meanwhile forcing the resulting distribution to be close to the sampling distribution, our generalized TEBC Maxent can be expected to alleviate the overfitting and underfitting. We also present a connection between TEB and Lidstone estimator. As a result, TEB-Lidstone estimator is developed by analytically identifying the rate of probability correction in Lidstone. Extensive empirical evaluation shows promising performance of both TEBC Maxent and TEB-Lidstone in comparison with various state-of-the-art density estimation methods.

Keywords Density estimation · Maximum entropy · Tsallis entropy · Tsallis entropy bias · Lidstone estimator
1 Introduction

The maximum entropy (Maxent) approach to density estimation was originally proposed by E. T. Jaynes [Jaynes, 1957], and since then has been widely used in many areas of computer science and statistical learning, especially natural language processing [Berger et al., 1996, Pietra et al., 1997]. The Maxent principle can be traced back to Jaynes’ classical description [Jaynes, 1957]:

“... the fact that a probability distribution maximizes entropy subject to certain constraints representing our incomplete information, is the fundamental property which justifies use of that distribution for inference; it agrees with everything that is known, but carefully avoids assuming anything that is not known.”

In implementing this principle, given a sampling distribution drawn from the underlying real distribution, Maxent computes a resulting distribution whose entropy is maximized, subject to a set of selected constraints. The standard Maxent can be formulated in Formula 1:

\[
\begin{align*}
\max_{P^{(m)}} & \quad S[P^{(m)}] \\
\text{st.} & \quad \sum_{j \in S_u} \bar{p}_j - a_u \leq \delta_u \quad \forall u \in U \\
& \quad \sum_{i \in S_c} \bar{p}_i = a^*_c \quad \text{or},
& \quad \sum_{i \in S_c} \bar{p}_i \geq a^*_c \quad \forall c \in C \\
& \quad \sum_{i \in S_u} \bar{p}_i \leq a^*_u
\end{align*}
\]

where \( P^{(m)} \equiv \langle \bar{p}_1, \ldots, \bar{p}_m \rangle \) is the resulting \( m \)-nomial probability distribution, \( S[\cdot] \) denotes the Shannon entropy of some probability distribution, \( C \) and \( U \) are two index sets, \( a^*_c, c \in C \) is the constant determined by reliable information, \( a_u \) and \( \delta_u, u \in U \) are the parameters that need to be empirically adjusted, and \( S_c, c \in C \) and \( S_u, u \in U \) are subsets of \( \{1, 2, \ldots, m\} \). Standard Maxent has two sets of constraints. The first set (indexed by \( C \)) includes all certain constraints, which are derived from reliable prior information and do not involve empirical parameters. For example, two of the most common certain constraints are \( \sum_{i \in S} \bar{p}_i = 1 \) and \( \bar{p}_i \geq 0 \). The second set (indexed by \( U \)) includes all uncertain constraints, which are from less reliable knowledge or sample information, and hence necessarily involve empirical parameters (e.g., \( a_u \) and \( \delta_u \)) to gain a satisfying performance. Note that there could be other specific forms of constraints not listed in Formula 1 e.g., the common form of real-valued feature functions. However, these constraint forms are essentially equivalent to and can be categorized into certain or uncertain constraints. Moreover, all certain and uncertain constraints considered in this paper are linear.

1.1 The Problem

Although the essential idea of Maxent is concise and elegant, the implementation of Maxent poses considerable practical complexity. Specifically, in a typical density esti-
information task, reliable prior information is often insufficient. In this case, if Maxent only involves certain constraints derived from reliable prior information, the resulting distribution will be away from the sampling distribution. Consequently, underfitting will result. Hence, Maxent usually involves a set of uncertain constraints, which force the resulting distribution to be close to the sampling distribution. The tolerable violation-level of the resulting distribution against the sampling distribution is controlled by a set of threshold parameters. These constraints and parameters are essentially empirical and ad-hoc. This is a dilemma: On one hand, if a large number of uncertain constraints and a set of tight threshold parameters are involved, the solution of Maxent will be close to the sampling distribution and might severely overfit the sample [Dudik et al., 2007]; On the other hand, if a small number of uncertain constraints or a set of loose threshold parameters are used, Maxent might underfit the sample and miss out some useful sample information.

1.2 Existing Work

In the framework of Maxent, main approaches to tackling overfitting or underfitting are parameter regularization and constraint relaxation. The former introduces some specific statistics (e.g., $l_1$, $l_2$, $l_1 + l_2$ etc.) as the regularized terms of the objective function and removes explicit constraints [Dudik et al., 2007; Chen and Rosenfeld, 2000; Lebanon and Lafferty, 2001; Late, 1994]. The latter aims to relax the constraints according to some theoretical considerations [Khudanpur, 1995; Kazama and Tsujii, 2003; Jedynak and Khudanpur, 2005; Jedynak and Khudanpur, 2005], e.g., Maximum Likelihood set in [Jedynak and Khudanpur, 2005]. The performance guarantee of some Maxent variants is rigorously established with respect to (w.r.t.) finite sample criteria, e.g., Probably Approximately Correct (PAC). However, according to our best knowledge, most of guarantees are, to some extent, self-referencing. For example, using log loss as the criterion, theoretical relations between the solution of Generalized Maxent (GME) and the best Gibbs distribution are given [Dudik et al., 2007]. However, the definition of the best Gibbs distribution intrinsically depends on the selection of feature functions. It turns out that, if the selection of feature functions is improper, the solution of GME might not be able to avoid overfitting or underfitting substantially even if it is close to the best Gibbs distribution.

1.3 Our Approach

In this paper, we propose a novel generalization of Maxent, under the framework of Tsallis entropy [Tsallis, 1988; Abe, 2000].

An important motivating observation is that, the expected Tsallis entropy of sampling distributions is always smaller than the Tsallis entropy of the underlying real distribution. To demonstrate this formally, we present a theoretical analysis on the expected Tsallis entropy bias (TEB) between sampling distributions and the underlying real distribution. The TEB is independent of the selection of constraints and can be

1 Please refer to Section 3.1 for more details about Tsallis entropy. For the sake of analytical simplicity, we only consider the Tsallis entropy with $q = 2$ [Tsallis, 1988] in this paper.

2 In this paper, the notation of “Tsallis entropy bias” has the same meaning as the “expected Tsallis entropy bias”. Accordingly, TEB has the “expected” sense in itself.

3 Actually, the TEB only depend on i.i.d. sampling presumption.
expressed by a simple closed-form formula of the sample size $n$ and the Tsallis entropy of the underlying real distribution. This observation naturally entails a quantitative re-interpretation and a theoretical guarantee of the Maxent principle: Since the entropy of sampling distributions is smaller, in the expected sense, than the entropy of the underlying real distribution, Maxent should increase the entropy of the sampling distribution to compensate the TEB and hence approximate the underlying real distribution. The TEB is first developed in the frequentist framework and we note it as Frequentist-TEB. In addition, by assuming a uniform Bayesian prior over all possible $m$-nomial distributions, a Bayesian-TEB is developed.

We argue that, in consistency with the basic principle of Maxent, a rigorously established compensation of Frequentist-TEB or Bayesian-TEB can help alleviate the overfitting problem. On the other hand, it is natural to overcome underfitting through simply forcing the resulting distribution to be close to the sampling distribution. By integrating these two strategies into our generalized Maxent, called Tsallis entropy bias compensation (TEBC) Maxent, it is expected that TEBC Maxent can alleviate overfitting and underfitting. Note that it is somewhat problematic to develop the similar method in the framework of Shannon entropy since a consistent and unbiased correction of Shannon entropy has not been exactly found yet, in general (see Section 2 for more details of the estimate of Shannon entropy).

In implementation, the TEBC Maxent is convex and hence can be efficiently solved. More importantly, TEBC Maxent can bypass the selection of uncertain constraints as well as parameter identification by introducing a parameter-free TEB constraint, aiming at quantitative entropy compensation.

In addition to the above Maxent framework, the generality of our theoretical results can be demonstrated by a practical connection between TEB and another widely used estimator, namely the Lidstone estimator. We will show that both Frequentist-TEB and Bayesian-TEB can offer guidance to identify the adaptive rate of probability correction, which needs to be empirically set in Lidstone. Accordingly, the so-called “F-Lidstone” and “B-Lidstone” estimators are derived respectively.

Extensive experimental results on a number of synthesized and real-world datasets demonstrate a promising performance of TEBC Maxent, F-Lidstone and B-Lidstone, in comparison with various state-of-the-art density estimation methods.

2 Related Work

The concept of maximum entropy has been existing in the Machine Learning literature for a long time and has resulted in various approaches. Its constrained form has been widely applied in many contexts [Berger et al., 1996, Kazama and Tsujii, 2003, Jedynak and Khudanpur, 2005]. Recently, there have been many studies of Maxent with $l_1$-style regularization [Khudanpur, 1992, Kazama and Tsujii, 2003, Williams, Ng, 2004, Goodman, 2004, Krishnapuram et al., 2003]. $l_2$-style regularization [Lau, 1994, Chen and Rosenfeld, 2000, Lebanon and Lafferty, 2001, Zhang, 2005] as well as some other types of regularization such as $l_1 + l_2$-style [Kazama and Tsujii, 2003], $l_2$-style regularization [Newman, 1977] and a smoothed version of $l_1$-style regularization [Dekel et al., 2003, Altun and Smola, 2006] derive duality and performance guarantees for settings in which the entropy is replaced by an arbitrary Bregman or Csiszar divergence. A thoroughly theoretic analysis of regularized Maxent can be found in [Dudik et al., 2007].
As another direction to density estimation, there are many smoothing methods that have been proposed in various contexts, e.g., information retrieval tasks [Zhai and Lafferty, 2001], speech recognition [Chen and Goodman, 1998] and cryptology [Good, 1953]. A typical family of general-purpose smoothing methods is Good-Turing estimator. All of them use the following equation to calculate the resulting frequencies of events:

$$F_X = \frac{(N_X + 1)}{E(N_X + 1)} \cdot \frac{E(N_X + 1)}{E(N_X)}$$

where $X$ is an event, $N_X$ is the number of times the event $X$ has been seen, within the sample of size $T$, and $E(n)$ is an estimate of how many different events that happened exactly for $n$ times. Different variants of Good-Turing estimator, e.g., the simplest Good-Turing estimator, Simple Good-Turing estimator [Gale and Sampson, 1995] and diminishing-attenuation estimator [Orlitsky et al., 2003], are based on different calculations of the $E(\cdot)$.

Another widely used smoothing method is Lidstone estimator [Chen and Goodman, 1998]. Typical variants of Lidstone estimator include Expected Likelihood Estimator, Laplace estimator and Add-tiny estimator. From a theoretical point of view, by defining the attenuation of a probability estimator as the largest possible ratio between the per-symbol probability assigned to an arbitrary sized sequence by any distribution and the corresponding probability assigned by the estimator, it can be shown that the attenuation of diminishing-attenuation estimators is unity [Orlitsky et al., 2003]. Note that the attenuation analysis is an asymptotic analysis w.r.t. large sample performance.

For the entropy correction, there are some methods to estimate the Shannon entropy bias. However, to the best of our knowledge, no consistent and unbiased correction of Shannon entropy has been developed. In principle, the "inconsistency" theorem leads to several approximations of the Shannon entropy bias [Milled, 1955, Carlton, 1969, Panzeri and Treves, 1994, Victor, 2000]. The analytical approximation of bias given by [Paninski, 2003] can be considered more rigorous than predecessors. However, this bias does not have a closed form and depends on specific prior distribution and the $c$ [Paninski, 2003], and hence it is hard to be computed in general. Regarding this, Paninski proposed an estimator, which is consistent even when the $c$ is bounded (provided that both $m$ and $n$ are sufficiently large) [Paninski, 2004]. However, a general and exact closed-form formula for Shannon entropy bias is still an open problem.

The rest of this paper is organized as follows: Section 3 gives a theoretical analysis on two crucial observations; Section 4 discusses the estimate of TEBs (Frequentist-TEB and Bayesian-TEB), introduces TEBC Maxent and reveals the connection between TEBs and Lidstone estimator; Section 5 gives two model-evaluating criteria; Experiments on synthesized and real-world datasets are constructed in Section 6 and the experimental results are reported and discussed. Finally, conclusions and future work are presented in Section 7.

3 Tsallis Entropy Bias

In this section, we present two theoretical observations, which motivate and underpin the proposed TEB, TEBC Maxent and TEB-Lidstone estimator.
3.1 Notations and Definitions

We use the following notations throughout the rest of the paper:

\[ P^{(m)} \equiv (p_1, \ldots, p_m) : \text{The underlying real } m\text{-nomial (} m \geq 2\text{)} probability distribution, where } \sum_{i=1}^{m} p_i = 1; \]

\[ \tilde{P}_{n}^{(m)} \equiv (\tilde{p}_1, \ldots, \tilde{p}_m) : \text{The sampling distribution of sample size } n \text{ w.r.t. } P^{(m)}, \text{where } \sum_{i=1}^{m} \tilde{p}_i = 1; \]

\[ \mathbb{P}^{(m)} : \text{The set of all possible } m\text{-nomial (} m \geq 2\text{)} probability distributions.} \]

\[ T_q \left[ P^{(m)} \right] \equiv k \frac{1 - \sum_{i=1}^{m} \tilde{p}_i^q}{q-1} : \text{The Tsallis entropy of } P^{(m)} \text{ w.r.t. the index } q, \text{where } k \]

is the Boltzmann constant; We have \( \lim_{q \to 1} T_q \left[ P^{(m)} \right] = k \cdot H \left[ P^{(m)} \right] \), where \( H \left[ P^{(m)} \right] \)

is the Shannon information entropy of \( P^{(m)} \).

The Tsallis entropy is the simplest entropy form that extends the Shannon entropy while maintaining the basic properties but allowing, if \( q \neq 1 \), nonextensivity [Santos and Math, 1997, Abe, 2000]. In this paper, for the sake of analytical convenience, we always assume \( q = 2 \) and neglect the subscript \( q \). In addition, without loss of generality, we omit the Boltzmann constant. It then turns out that \( T \left[ P^{(m)} \right] = 1 - \sum_{i} \tilde{p}_i^2 \).

3.2 Main Results

**Proposition 1** Given an arbitrary \( m\)-nomial probability distribution \( P^{(m)} \in \mathbb{P}^{(m)} \), let \( \tilde{P}_{n}^{(m)} \) be the sampling distribution of sample size \( n \) with respect to \( P^{(m)} \), \( E_{P,n}^{(m)} (T) \) be the expected Tsallis entropy of \( \tilde{P}_{n}^{(m)} \), and \( T \left[ P^{(m)} \right] \) be the Tsallis entropy of \( P^{(m)} \), then

\[
E_{P,n}^{(m)} (T) = \frac{n - 1}{n} T \left[ P^{(m)} \right] \tag{2}
\]

**Proof** Let \( P^{(m)} = \left\langle p_1, \ldots, p_{m-1}, 1 - \sum_{i=1}^{m-1} p_i \right\rangle \) be an \( m\)-nomial probability distribution. Denote the set of all possible sampling distributions of sample size \( n \) as

\[ \mathbb{S}_n^{(m)} \equiv \left\{ \tilde{P}_{n}^{(m)} \equiv \left\langle \frac{x_1}{n}, \ldots, \frac{x_{m-1}}{n}, \frac{n - \sum_{i=1}^{m-1} x_i}{n} \right\rangle \mid x_1, \ldots, x_{m-1} \in \mathbb{N}, x_1 + \ldots + x_{m-1} \leq n \right\} \]

where \( x_i \) is the count of the \( i \)th nomial. Given \( P^{(m)} \), the occurrence probability of a sampling distribution \( \tilde{P}_{n}^{(m)} \equiv \left\langle \frac{x_1}{n}, \ldots, \frac{x_{m-1}}{n}, \frac{n - \sum_{i=1}^{m-1} x_i}{n} \right\rangle \in \mathbb{S}_n^{(m)} \) is given by the following equation:

\[
\Pr \left[ \tilde{P}_{n}^{(m)} \mid P^{(m)} \right] = \frac{n!}{(n - \sum_{i=1}^{m-1} x_i)! \prod_{i=1}^{m-1} x_i!} \left( 1 - \sum_{i=1}^{m-1} \tilde{p}_i \right)^{n - \sum_{i=1}^{m-1} x_i} \prod_{i=1}^{m-1} \tilde{p}_i^{x_i} \tag{3}
\]

Note that we assume \( \theta^0 = 1 \) in Formula (3). Hence, we have

\[
E_{P,n}^{(m)} (T) = \sum_{x_1=0}^{n} \sum_{x_2=0}^{n-x_1} \ldots \sum_{x_{m-1}=0}^{n-x_1-x_2-\ldots-x_{m-2}} T \left[ \tilde{P}_{n}^{(m)} \right] \cdot \Pr \left[ \tilde{P}_{n}^{(m)} \mid P^{(m)} \right]
\]
By the definition of Tsallis entropy \((q = 2)\), we have

\[
T\left[p^{(m)}_n\right] \equiv 1 - \sum_{i=1}^{m} \left(\frac{x_i}{n}\right)^2
\]

where we denote \(n - \sum_{i=1}^{m-1} x_i\) as \(x_m\). It is convenient to express \(E_{P,n}^{(m)}(T)\) as the following:

\[
E_{P,n}^{(m)}(T) = 1 - \sum_{i=1}^{m} E_{P,n}^{(m)}\left(\frac{x_i}{n}\right)^2
\]

where

\[
E_{P,n}^{(m)}\left(\frac{x_i}{n}\right)^2 \equiv \sum_{x_1=0}^{n} \sum_{x_2=0}^{n-x_1} \cdots \sum_{x_{m-1}=0}^{n-x_1-\cdots-x_{m-2}} \left(\frac{x_i}{n}\right)^2 \cdot \Pr\left(P^{(m)}_n \mid p^{(m)}\right), \quad i = 1 \ldots m
\]

Note that \(E_{P,n}^{(m)}(x_i^2)\) is just the moments about the origin of the multinomial distribution and given by \(E_{P,n}^{(m)}(x_i^2) = n(n-1)p_i^2 + np_i\). Hence, we have \(E_{P,n}^{(m)}\left(\frac{x_i}{n}\right)^2 = \frac{(n-1)p_i^2 + p_i}{n}\).

It turns out that

\[
E_{P,n}^{(m)}(T) = 1 - \sum_{i=1}^{m} \left(\frac{n-1}{n}\right) p_i^2 + p_i = \frac{n-1}{n} \left(1 - \sum_{i=1}^{m} p_i^2\right)
\]

The r.h.s of the last equation is just \(T[p^{(m)}]\).

**Corollary 1**

\[
\lim_{n \to \infty} E_{P,n}^{(m)}(T) = T[p^{(m)}] \quad (4)
\]

**Proof** The corollary follows immediately from Formula(3).

The above result is developed in the frequentist framework and hence corresponds to a Frequentist-TEB. In the following, a uniform Bayesian TEB (Bayesian-TEB for short) is developed by assuming a uniform Bayesian prior over all possible \(m\)-nominal distributions.4

**Proposition 2**

Given the uniform probability metric over \(p^{(m)}\), the expectation of \(E_{P,n}^{(m)}\), i.e. \(E_n^{(m)}\), is given by

\[
E_n^{(m)}(T) = \frac{(n-1) \cdot (m-1)}{n \cdot (m+1)} \quad (5)
\]

**Proof** By the definition of mathematical expectation, we have

\[
E_n^{(m)}(T) = \frac{1}{Z^{(m-1)}} \int_{0}^{1} \int_{0}^{1-p_1} \cdots \int_{0}^{1-\sum_{i=1}^{m-2} p_i} E_{P,n}^{(m)}(T) \, dp_{m-1} dp_{m-2} \cdots dp_1
\]

where \(Z^{(m-1)}\) is the normalization factor determined by the \((m-1)\)-order integral operator,

\[
Z^{(m-1)} = \int_{0}^{1} \int_{0}^{1-p_1} \cdots \int_{0}^{1-\sum_{i=1}^{m-2} p_i} dp_{m-1} dp_{m-2} \cdots dp_1 = \frac{1}{(m-1)!}
\]

4 The code package for the numeric evaluation of Proposition 1 and 2 is provided at [http://www.comp.rgu.ac.uk/staff/pz/TEBC/PropositionValidationCodes.zip](http://www.comp.rgu.ac.uk/staff/pz/TEBC/PropositionValidationCodes.zip)
Expands and rewrites $E_{P,n}^{(m)}(T)$ as the following:

$$E_{P,n}^{(m)}(T) = \frac{2(n-1)}{n} \left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right)$$ \hspace{1cm} (6)

Hence, we have

$$L_n^{(m)}(T) = \frac{2(n-1)}{Z^{(m-1)} - n} \int_0^1 \int_0^{1-p_1} \cdots \int_0^{1-\sum_{i=1}^{m-2} p_i} \left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right) \ dp_{m-1} dp_{m-2} \cdots dp_1$$ \hspace{1cm} (7)

To simplify the notations, we define the $(m-1)$-order integral operator:

$$L^{(m-1)} = \int_0^1 \int_0^{1-p_1} \cdots \int_0^{1-\sum_{i=1}^{m-2} p_i} \ dp_{m-1} dp_{m-2} \cdots dp_1$$

We denote $L^{(m-1)}(f(p_1, \ldots, p_{m-1}))$ as

$$L^{(m-1)}(f(p_1, \ldots, p_{m-1})) \equiv \int_0^1 \int_0^{1-p_1} \cdots \int_0^{1-\sum_{i=1}^{m-2} p_i} f(p_1, \ldots, p_{m-1}) \ dp_{m-1} dp_{m-2} \cdots dp_1$$

Then the proof of Formula (6) is reduced to solve the closed-form of

$$L^{(m-1)} \left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right)$$

Due to the symmetry of integral domain, $L^{(m-1)}$ has the following properties:

(a) $L^{(m-1)}(p_i) = L^{(m-1)}(p_j), 1 \leq i, j \leq m - 1$

(b) $L^{(m-1)}(p_i^2) = L^{(m-1)}(p_j^2), 1 \leq i, j \leq m - 1$

(c) $L^{(m-1)}(p_i \cdot p_j) = L^{(m-1)}(p_k \cdot p_l), 1 \leq i, j \leq m - 1, i \neq j, k \neq l$

Therefore, if the general term formulae of $L^{(m-1)}(p_i)$, $L^{(m-1)}(p_i^2)$ and $L^{(m-1)}(p_i \cdot p_j)$, $i \neq j$, and their term numbers are available, the general term formula of $E_{n}^{(m)}(T)$ could be obtained directly.

The following general term formulae can be verified:

(a') $L^{(m-1)}(p_i) = \frac{1}{m!}$

(b') $L^{(m-1)}(p_i^2) = \frac{2}{(m+1)!}$

(c') $L^{(m-1)}(p_i \cdot p_j) = \frac{1}{(m+1)!}$

then

$$E_{n}^{(m)}(T) = \frac{2(n-1)}{Z^{(m-1)} - n} \cdot L^{(m-1)} \left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right)$$

$$= \frac{2(n-1)}{Z^{(m-1)} - n} \left[ \frac{m-1}{m!} - \frac{2(m-1)}{(m+1)!} \right]$$

Recall that $Z^{(m-1)} = \frac{1}{(m-1)!}$, and after some simplification steps, Formula (6) is obtained from the above equation, which completes the proof of Proposition 2.
Corollary 2 Let \( E(m) (T) = \frac{1}{Z^{(m-1)}} \int_0^1 \cdots \int_0^1 \cdots \int_0^1 \int_0^1 \cdots \int_0^1 \cdots \int_0^1 \cdots \int_0^1 \cdots \int_0^1 T \left[ p^{(m)} \right] dp_{m-1} dp_{m-2} \cdots dp_1, \)
where \( Z^{(m-1)} \) is the normalization factor \( \frac{1}{(m-1)!} \). Then we have
\[
\lim_{n \to \infty} E_n^{(m)} (T) = E^{(m)} (T)
\]
Proof The corollary follows directly from the fact that \( E^{(m)} (T) \) can be given by the r.h.s of Formula 2 except for a multiplicative factor \( \frac{n-1}{n} \).

4 Density Estimate based on Tsallis Entropy Bias

Based on the above theoretic results, we first discuss the issue on the estimate of Tsallis entropy bias, and then propose density estimate methods in Maxent framework and Lidstone framework, respectively.

4.1 On Estimation of Tsallis Entropy Bias

To apply the result of Proposition 1, the frequentist Tsallis entropy bias (Frequentist-TEB) should be effectively estimated so that the Tsallis entropy of the sampling distribution \( \hat{P}^{(m)}_n \) can be compensated accordingly. According to Formula 2, the expected Tsallis entropy of \( \hat{P}^{(m)}_n \), i.e., \( E_{P,n}^{(m)} (T) \), is \( (n-1)/n \) of the Tsallis entropy of the underlying real distribution \( P^{(m)} \), i.e., \( T \left[ P^{(m)} \right] \). We denote the estimation of \( E_{P,n}^{(m)} (T) \) as \( \hat{E}_{P,n}^{(m)} (T) \), then \( \frac{n}{n-1} \hat{E}_{P,n}^{(m)} (T) \) can be considered as an estimation of \( T \left[ \hat{P}^{(m)}_n \right] \). Hence, the estimation of frequentist Tsallis entropy bias, i.e. Frequentist-TEB, is given by
\[
\Delta T = \frac{n}{n-1} \hat{E}_{P,n}^{(m)} (T) - T \left[ \hat{P}^{(m)}_n \right]
\]
The simplest (and unbiased) estimation of \( \hat{E}_{P,n}^{(m)} (T) \) is given by \( T \left[ \hat{P}^{(m)}_n \right] \), and hence the corresponding estimated TEB is given by
\[
\Delta T = \frac{1}{n-1} T \left[ \hat{P}^{(m)}_n \right]
\]
Remark 1 \( T \left[ \hat{P}^{(m)}_n \right] \) is an unbiased estimate of \( E_{P,n}^{(m)} (T) \). Therefore, Formula 10 gives an unbiased correction of \( T \left[ P^{(m)} \right] \). In addition, the consistency of this correction follows from the law of large numbers (if \( m \) is finite) or central limit theorem for multinomial sums [Morris, 1975] (if \( m \) is infinite).

Surprisingly, experimental results (detailed in Section 6) show the TEBC Maxent and TEB-Lidstone estimator based on this naive estimator can outperform all comparative density estimation models in most cases.

In many cases, using statistical re-sampling techniques, e.g., Bootstrap [Wasserman, 2006], we can achieve more accurate estimations of \( T \left[ P^{(m)} \right] \), and hence obtain better estimations of Frequentist-TEB. In the following, we give an estimation procedure of \( T \left[ P^{(m)} \right] \), which is optimal in the sense of the least squared error.
Let us rewrite Formula \(2\) so that \(E_{P,n}^{(m)}(T)\) is expressed by a function of \(n\)

\[
E_{P,n}^{(m)}(T) = K \cdot \frac{n - 1}{n}
\]

where \(K\) is a constant slope and determined by \(T \left[ p^{(m)} \right] \). We can estimate \(E_{P,i}^{(m)}(T)\), \(1 \leq i \leq n\) by re-sampling techniques and obtain \(\hat{E}_{P,i}^{(m)}(T)\), \(1 \leq i \leq n\). Note that the re-sampling is meaningful only if \(i < n\). The remaining task is to solve an unconstrained quadratic program so that the squared error

\[
\sum_{i=1}^{n} \left( \hat{E}_{P,i}^{(m)}(T) - \frac{i - 1}{i} K \right)^2
\]

is minimized. This minimum corresponds to the zero point of the first derivative in the cost function

\[
0 = \frac{\partial}{\partial K} \sum_{i=1}^{n} \left( \hat{E}_{P,i}^{(m)}(T) - \frac{i - 1}{i} K \right)^2
\]

By expanding the above equation, it turns out that the estimated slope is given by

\[
\hat{K} = \frac{\sum_{i=1}^{n} (i - 1)/i \cdot \hat{E}_{P,i}^{(m)}(T)}{\sum_{i=1}^{n} (i - 1)^2/i^2}
\]

where \(\hat{K}\) is the estimation of \(T \left[ p^{(m)} \right] \). Note that, in practice, it is often sufficient to only involve an appropriate subset of \(\hat{E}_{P,i}^{(m)}(T)\), \(1 \leq i \leq n\), in the cost function \((11)\) to construct the estimate of \(T \left[ p^{(m)} \right] \).

However, even with the re-sampling technique, in the case that the sampling is seriously inadequate, it seems still difficult to estimate \(E_{P,n}^{(m)}(T)\) accurately, which might in turn result in inaccurate Frequentist-TEB. In this case, some Bayesian prior over the space of all possible real distributions might be more useful. The results of Proposition \(2\) and Corollary \(2\) guide the construction of uniform Bayesian-TEB, i.e.,

\[
\Delta T = \frac{m - 1}{n \cdot (m + 1)}
\]

by assuming the uniform probability metric over all possible real distributions. Note that uniform Bayesian-TEB is directly obtained by computing the difference between the expected Tsallis entropy of all possible real distributions and the expectation of \(E_{P,n}^{(m)}(T)\), i.e. \(E_{n}^{(m)}(T)\), w.r.t. uniform prior. Hence, it avoids the estimation of \(E_{P,n}^{(m)}(T)\).

**Remark 2** Corollary \(2\) shows that \(E_{n}^{(m)}(T)\) is the asymptotically unbiased estimate of \(E^{(m)}(T)\) and can be unbiased if the Bayesian-TEB \(\frac{m - 1}{n(m + 1)}\) is compensated. In addition, this corrected estimator is also consistent with \(E^{(m)}(T)\).

In summary, Remark1 and Remark2 show that the estimates of the Tsallis entropy bias, w.r.t both Frequentist and Bayesian frameworks, can be considered sound in the sense of unbiasedness and consistency. Note that the Shannon entropy estimate lacks these guarantees.
4.2 TEBC Maxents

In this subsection, we propose three Tsallis entropy bias compensation (TEBC) Maxents to compute resulting distributions. These distributions are most similar to the sampling distribution w.r.t. different similarity criteria, subject to the constraint that the estimated Frequentist/Bayesian-TEB, denoted as $\Delta T$, is forcibly compensated. This strategy can help to alleviate the overfitting and underfitting problems.

Given any $m$-nomial sampling distribution $\hat{P}_n(m) \equiv (\hat{p}_1, \ldots, \hat{p}_m)$ of sample size $n$ and the estimated $\Delta T$, the TEBC Maxents can be constructed to compute the resulting distribution $\bar{P}(m) \equiv (\bar{p}_1, \ldots, \bar{p}_m)$ w.r.t. the criterion of $l^2$ norm, Jensen-Shannon (JS) divergence (see Formula 15 for details) or Maximum Likelihood, respectively:

**Model 1: $l^2$ Tsallis Entropy Bias Compensation ($l^2$-TEBC)**

$$\min_{\hat{P}_n(m)} \sum_{i=1}^{m} (\bar{p}_i - \hat{p}_i)^2$$

s.t. $T[\bar{P}(m)] \geq T[\hat{P}_n(m)] + \Delta T$

(13)

**Model 2: JS-Divergence Tsallis Entropy Bias Compensation (JSD-TEBC)**

$$\min_{\hat{P}_n(m)} JSD[\bar{P}(m) \bigg| \hat{P}_n(m)]$$

s.t. $T[\bar{P}(m)] \geq T[\hat{P}_n(m)] + \Delta T$

(14)

where $JSD[\cdot | \cdot]$ denotes the JS-divergence.

Note that a common statistic to measure the divergence between two probability distributions is the Kullback-Leibler (KL) divergence. Despite of the computational and theoretical advantages of KL-divergence, it is not symmetric in its arguments. Reversing the arguments in the KL-divergence function can yield substantially different results. Furthermore, $KL(P, Q)$ may be seriously underestimated if $P$ involves zero terms since $\lim_{p_i \to 0} p_i \log \frac{p_i}{q_i} = 0$. Besides, $KL(P, Q)$ is sensitive to penalty terms used in the case of $q_i = 0$. Hence, we apply a symmetrized variant of KL-divergence, i.e., JS-divergence, instead.

$$JSD[P | Q] \equiv \frac{1}{2} D[P | M] + \frac{1}{2} D[Q | M]$$

(15)

where $D[P | M]$ is the KL-divergence from $P$ to $M$ and $M = (P + Q)/2$.

**Model 3: Maximum Likelihood Tsallis Entropy Bias Compensation (ML-TEBC)**

$$\max_{\hat{P}_n(m)} \log \left\{ Pr\left[\hat{P}_n(m) \bigg| \bar{P}(m)\right]\right\}$$

s.t. $T[\bar{P}(m)] \geq T[\hat{P}_n(m)] + \Delta T$

(16)

where $Pr\left[\hat{P}_n(m) \bigg| \bar{P}(m)\right]$ is given by Formula 3.

In Models 1, 2 and 3, all objective functions aim at forcing the resulting distribution similar to sampling distribution as well as possible. This is to counter the underfitting
problem. Meanwhile, the TEB constraint is used to increase the entropy of the resulting distribution and then compensate the Tsallis entropy bias, in order to make the resulting distribution approximate the underlying real distribution. This is to avoid the overfitting problem. From another point of view, in the expected sense, the objective function aims at reducing the Tsallis entropy, while the TEB constraint is adopted to necessarily increase the Tsallis entropy. Through this joint effort, the objective function forces the TEB constraint to hold as equality, which is consistent with our previous theoretical analysis.

In implementation, all the above objective functions and constraints are convex. Therefore, TEBC Maxents can be globally solved by efficient methods, e.g., the interior method [Boyd and Vandenberghe, 2004]. In specific application contexts, TEBC Maxents should include certain constraints, which are derived from reliable prior information and do not involve empirical threshold parameters. A specific example on the form of certain constraints is given in our experiment (see Section 6.2.2 for details). TEBC Maxents can be constructed with Frequentist-TEB or Bayesian-TEB. In the cases that sampling process is seriously inadequate, the Bayesian TEBC Maxents are expected to have stable performance. The cause is that, given uniform Bayesian prior and an inadequate sampling, e.g., \( n \approx m \), the standard deviation of \( E_{P,m}^{(m)}(T) \) tends to be negligible compared to uniform Bayesian-TEB, which implies a relatively stable estimation of uniform Bayesian-TEB. The detailed proof is given in Proposition 3 of Appendix A.

4.3 TEB-Lidstone Estimators

There is a natural connection between TEBs and Lidstone estimator. Lidstone’s law of succession suggests the family of Lidstone estimators in the following form:

\[
\hat{p}_i = \frac{x_i + f}{n + f \cdot m}
\]

where \( n \) is the sample size, \( m \) is the number of nominals, \( x_i \) is the count of the \( i \)th nominal and \( f \) is a parameter indicating the rate of probability correction (normally between 0 and 1). When \( f = 0.5 \), it turns out to be the well-known Expected Likelihood Estimator (ELE), i.e.,

\[
\hat{p}_i = \frac{x_i + 0.5}{n + 0.5 \cdot m}
\]

Another two common Lidstone estimators are add-one estimator \( (f = 1) \) and add-tiny estimator \( (f = 1/n) \). The smaller \( f \) is, the less probability mass it compensates for underestimations. There exist some explanations on the selection of parameter \( f \). For example, ELE gives a Bayesian justification by assuming a uniform prior for a binomially distributed variable [Box and Tiao, 1973]. However, in general cases, \( f \) is empirically configured.

TEBs offer a set of criteria, either of which analytically identifies an adaptive \( f \) w.r.t. a specific input sample, and derives the TEB-Lidstone estimator. The fundamental idea is to solve such an \( f \) so that the Tsallis entropy bias of the input sample is quantitatively compensated. That is

\[
1 - \sum_i \left( \frac{x_i + f}{n + f \cdot m} \right)^2 = T \left[ \hat{P}_0^{(m)} \right] + \Delta T
\]
where $\Delta T$ can be Frequentist-TEB or Bayesian-TEB. Let $\alpha \equiv 1 - \left( T \left( \hat{P}^{(m)}_n \right) + \Delta T \right)$. It turns out that we have the following quadratic equation in the single variable $f$:

$$
\left( \alpha m^2 - m \right) f^2 + 2n \left( \alpha m - 1 \right) f + \left( kn^2 - \sum_{i=1}^{m} x_i^2 \right) = 0 \quad (17)
$$

Occasionally, Formula (17) has not real roots. In this case, we can simply select $f$ corresponding to the minimum (if $\alpha m^2 - m > 0$) or the maximum (if $\alpha m^2 - m < 0$) of the l.h.s of Formula (17). Consequently, the so-called “F-Lidstone” and “B-Lidstone” estimators are derived on Frequentist-TEB and Bayesian-TEB, respectively.

Note that, in principle, the Tsallis entropy bias can also serve to identify the parameters of some other estimators, e.g., the multiplicative parameter of Good-Turing estimator. We omit the computation details here.

5 Evaluation Criteria

The performance of a density estimation method can be directly evaluated by measuring the similarity between its solution and the underlying real distribution. As mentioned in Formula (15), JS-divergence can be considered as a candidate criterion. In addition, we use the expected log loss (the expect negative normalized log likelihood [Dudik et al., 2007]) as another similarity criterion. The log loss of a resulting distribution $P^{(m)} \equiv \langle \hat{p}_1, \ldots, \hat{p}_m \rangle$ with respect to the sample $x \equiv \langle x_1, x_2, \ldots, x_m \rangle$ is defined as:

$$
L_{P^{(m)}} (x) \equiv - \log \hat{p}_1^{x_1} \hat{p}_2^{x_2} \cdots \hat{p}_m^{x_m} = - \sum_{i=1}^{m} x_i \log \hat{p}_i \quad (18)
$$

Recall that, given a underlying real $m$-nomial distribution $P^{(m)} \equiv \langle p_1, \ldots, p_m \rangle$, the occurrence probability of a sample $x \equiv \langle x_1, x_2, \ldots, x_m \rangle$ of size $n$ can be expressed by

$$
\Pr \left[ x \left| P^{(m)} \right. \right] = \frac{n!}{x_1! x_2! \cdots x_m!} \cdot p_1^{x_1} p_2^{x_2} \cdots p_m^{x_m} \quad (19)
$$

Hence, we can define the expected log loss of $P^{(m)}$ w.r.t. $P^{(m)}$ as

$$
E_L \left[ \hat{P}^{(m)} \left| P^{(m)} \right. \right] \equiv \sum_{x \in X} L_{P^{(m)}} (x) \Pr \left[ x \left| P^{(m)} \right. \right] \quad (20)
$$

where $X$ stands for the set of all possible samples of size $n$. By substituting the r.h.s of Formula (20) by Formula (18) and (19) it can be checked that

$$
E_L \left[ \hat{P}^{(m)} \left| P^{(m)} \right. \right] = \sum_{x \in X} \sum_{i=1}^{m} -x_i \log \hat{p}_i \cdot \frac{n!}{x_1! x_2! \cdots x_m!} \cdot p_1^{x_1} p_2^{x_2} \cdots p_m^{x_m}
$$

$$
= - \sum_{i=1}^{m} \log \hat{p}_i \sum_{x \in X} x_i \cdot \frac{n!}{x_1! x_2! \cdots x_m!} p_1^{x_1} p_2^{x_2} \cdots p_m^{x_m}
$$

$$
= - \sum_{i=1}^{m} \log \hat{p}_i \left( n p_i \right) = -n \sum_{i=1}^{m} \log \hat{p}_i \quad (21)
$$

To more systematically measure the performance of different algorithms w.r.t a specific evaluation criterion, we introduce the Performance Score (PS) as below:
\[ P_{SD}(A) = \frac{C_D(A) - C_D(Worst)}{C_D(Best) - C_D(Worst)} \]  

where \( A \) stands for an algorithm under evaluation, \( C \) represents an evaluation criterion and \( D \) denotes a specific dataset; the performance value \( C_D(A) \) is evaluated by criterion \( C \) for algorithm \( A \) running on dataset \( D \), and \( C_D(Best) \) and \( C_D(Worst) \) are the performance values of the best and worst algorithms on \( D \), respectively.

6 Experiments

In this section, we construct three sets of experiments. First, if reliable prior information is available, in Maxent framework, TEBC Maxents’ performance will be evaluated in comparison with standard Maxent, GME (a \( l_1 \)-regularized Maxent which has PAC guarantee of performance) \cite{Dudik2007}, as well as Maxents based on Shannon entropy bias (SEB) \cite{Miller1955} which is described in Section 6.2.1. Second, in case that reliable prior information is not available, we will verify the effectiveness of TEB-Lidstone, by comparing their performance with comparative Lidstone and Good-Turing estimators, together with SEB-Lidstone which is derived from the above SEB in a similar way to TEB-Lidstone (described in Section 6.3.1). In all the above experimental settings, both synthesized and real-world datasets are employed. For TEBs, Bayesian-TEB is calculated by Formula 12, and Frequentist-TEB is estimated by the naive estimator given in Formula 10, which is more efficient in large-scale experiments and also can give a satisfying performance in both Maxent and Lidstone frameworks.

6.1 Datasets Description

First, synthesized probability distributions are generated to serve as the underlying real \( m \)-nomial distributions \( p(m) \). To this end, we adopt a simple Monte Carlo method to randomly draw \( m \) positive points from a source distribution, and then normalize them to form an underlying real distribution. The source distributions we used include uniform distribution \( U(0,1) \), the absolute value of standard normal distribution \( |N(0,1)^2| \), normal distribution \( N(3,1^2) \), \( \chi^2 \) distribution \( \chi^2(10) \), binomial distribution \( B(30,0.2) \) and beta distribution \( \beta(3,6) \). After the underlying real distribution is generated, a sample of size \( n \) is drawn from it, which can be then used to calculate the sampling distribution \( \hat{p}(m) \).

We also adopt four real-world datasets: UCI-Dexter, UCI-Statlog, UCI-ISOLET and UCI-Sonar, in order to generate the underlying real distributions.

Text dataset: Dexter

\[ \text{http://www.comp.rgu.ac.uk/staff/pz/TEBC/TEB_Experiment_Codes.zip} \]

\[ \text{http://archive.ics.uci.edu/ml/machine-learning-databases/dexter/DEXTER/} \]

\[ \text{http://archive.ics.uci.edu/ml/machine-learning-databases/statlog/satimage/} \]

\[ \text{http://archive.ics.uci.edu/ml/machine-learning-databases/isolet/} \]

\[ \text{http://archive.ics.uci.edu/ml/machine-learning-databases/undocumented/connectionist-bench/sonar/} \]
UCI-Dexter is a text dataset, containing 2000+300 documents. Each document is represented as a 20000-term count vector. Before the text dataset is actually employed, it is preprocessed by dropping the terms that occur too frequently, i.e., the “stop words”. After the preprocessing step, \( m \) terms could be randomly selected from the whole term set and the frequencies of these selected terms are considered as the underlying real distribution \( P(m) \). Then, we randomly choose a bag (size \( n \)) of words from all the documents as a sample. The frequencies of these terms in the sample are calculated and considered as the sampling distribution \( \hat{P}(m) \).

Non-text datasets: Statlog, ISOLET, Sonar

UCI-Statlog (Landsat Satellite) dataset consists of all possible \( 3 \times 3 \) neighborhoods in a \( 82 \times 100 \) pixel sub-area of a single scene which is represented by four digital images in different spectral bands. A sample is then defined as the pixel values of each \( 3 \times 3 \) neighborhood in the four spectral bands (hence \( 4 \times 9 = 36 \) features in total). The size of the dataset is 4435+2000.

UCI-ISOLET dataset includes 150 subjects speaking the name of each letter of the alphabet twice. The speakers are divided into groups of 30 speakers. There are 617 real-value features including spectral coefficients, contour features, sonorant features, pre-sonorant features, and post-sonorant features but in an unknown order.

UCI-Sonar contains 111 patterns obtained by bouncing sonar signals off a metal cylinder at various angles and under various conditions, and 97 patterns obtained from rocks under similar conditions. The transmitted sonar signal is a frequency-modulated chirp, rising in frequency. The data set contains signals obtained from a variety of different aspect angles, spanning 90 degrees for the cylinder and 180 degrees for the rock. Each pattern is a set of 60 numbers in the range 0.0 to 1.0. Each number represents the energy within a particular frequency band, integrated over a certain period of time.

For the above three non-text datasets, in order to generate the \( m \)-nomial underlying real distribution, we simply partition a randomly selected feature into \( m \) intervals covering the whole range of this single feature. Then the number of instances in each interval is counted and finally the underlying real distribution \( P(m) \) is formed by normalizing the count vector. The sampling process is to first randomly choose \( n \) instances and distribute them into the corresponding intervals based on their feature value, and then form the sampling distribution \( \hat{P}(m) \) by normalizing this sampling count vector.

6.2 TEBC Maxents vs. Comparative Maxents

Maxent is widely used due to its effective use of reliable prior information. In this set of experiments where the reliable prior information is given, TEBC Maxents and other Maxents are compared in terms of their density estimation performance.

6.2.1 Maxents

Various forms of Maxents are tested, including Frequentist TEBC Maxents (\( F-\ell_2^2 \)-TEBC, F-ML-TEBC and F-JSD-TEBC), Bayesian TEBC Maxents (\( B-\ell_2^2 \)-TEBC, B-ML-TEBC and B-JSD-TEBC), standard Maxent (SME for short), and GME [Dudik et al., 2007] (implemented by \( \ell_1 \)-SUMMET and \( \ell_1 \)-PLUMMET, which stand for selective-update and parallel-update algorithms for \( \ell_1 \)-regularization Maxent, respectively). In addition, we also construct three Maxents based on Shannon entropy bias (SEB) [Miller, ]
SEB Maxents are similar to TEBC Maxent (Model 1-3) except that the TEB constraint is replaced by the following SEB constraint:

\[
S \left[ \tilde{P}(m) \right] \geq S \left[ \hat{P}(m) \right] + \Delta S
\]  

(23)

where \( S[\cdot] \) denotes the Shannon entropy of some probability distribution and \( \Delta S = (m - 1)/(2n) \) denotes SEB\(^{10} \). We use \( \frac{m-1}{2n} \) as the correction since it is simple in form and frequently-used. Note that it cannot be considered an unbiased correction, in a strict sense [Paninski, 2003]. By substituting the SEB constraint for the TEB constraint in Model 1-3, three new Maxents are introduced in the experiment, namely \( L^2 \)-SEB, ML-SEB and JSD-SEB.

Note that in the following, we adopt “Sample” to represent the method using the sampling distribution as the resulting distribution directly.

6.2.2 Certain and Uncertain Constraints

Two kinds of constraints are involved. One is certain constraints, and the other is uncertain constraints. Certain constraints are derived from reliable prior information, which is incomplete information of the underlying real distribution. Specifically, certain constraints can be represented by a set of constraints as follows:

\[
\sum_{i \in S_c} \bar{p}_i = a_c^* = \sum_{i \in S_c} \hat{p}_i \quad \forall c \in C
\]

(24)

where \( S_c \) is a subset of \( \{1, 2, \ldots, m\} \). In order to form this subset, we randomly choose a number \(|S_c|\) from \( \{1, 2, \ldots, m - 1\} \), and then randomly select \(|S_c|\) indexes from \( \{1, 2, \ldots, m\} \). If we do this step \( k \) times, \( k \) certain constraints can be derived, and then the set \( C \) of all certain constraints is formed.

Uncertain constraints are derived from sampling information, together with empirical threshold parameters to control the similarity between the resulting distribution and the sampling distribution. Specifically, for every \( i \), if \( \hat{p}_i \geq \text{th} \), then we construct an uncertain constraint represented by Box Constraint:

\[
|\bar{p}_i - \hat{p}_i| \leq \delta
\]

(25)

where \( \delta \) and \( \text{th} \) are threshold parameters. In our experiments, we fix \( \text{th} \) as \( 0.2/m \), and adjust \( \delta \) to find relatively optimal performance for standard Maxent and GME.

6.2.3 Parametric Configuration

For all the models, the same parameters are used, including generating times, bin number, sample size, and sampling times. Generating times is the number of times to generate the underlying real distribution. Sampling times is the number of times to draw the sampling distribution from the given underlying real distribution. Note that in order to avoid the zero probability of any bin in the \( m \)-nomial underlying real distribution, the bin number \( m \) should be set properly for each real-world dataset in terms of its scale. For example, Sonar dataset has a relatively small number of data

\(^{10} \) In the original formula, an estimate of \( m \) is used instead of the real one. In our context, \( m \) is known in advance and hence the estimation can be avoided.
points. Therefore, we let $m_{\text{Sonar}} = 30$ to avoid a degenerated $m$-nomial underlying real distribution.

All Maxents involve the same certain constraints. TEBC Maxents and SEB Maxents adopt the corresponding TEB and SEB constraints, while other three Maxents use uncertain constraints. For uncertain constraints, we choose $\delta$ in Formula 25 from $[1 \times 4, 1.6e^{-3}]$ with increment $1 \times 4$. The performance of TEBC Maxents will be compared with the performance of comparative Maxents with the optimal $\delta$. Under this optimal $\delta$, comparative Maxents can obtain relatively optimal performance compared with the performance using other $\delta$’s. The parametric configuration is listed in Table 1.

| Category                          | Detailed Configurations                                                                 |
|-----------------------------------|----------------------------------------------------------------------------------------|
| Generating Times                  | $r = 10$                                                                                |
| $#\text{Bin}$                     | $m_{\text{Syn, Dexter, ISOLET}} = 100$                                                 |
|                                  | $m_{\text{SAT}} = 50$, $m_{\text{Sonar}} = 30$                                        |
| Sample Size                       | $n = 10 \cdot m$                                                                       |
| Sampling Times                    | $s = 20$                                                                               |
| $#\text{Certain Constraints}$     | $k = 0.2 \times m$, $k = 0.05 \times m$                                               |
| Threshold parameter $\delta$      | $6 \times 4 \text{ chosen from } [1 \times 4, 1.6e^{-3}]$                             |

Table 1 Parametric Configuration in Maxent Framework

6.2.4 Results

We employ the parametric configuration in Table 1 to run every Maxent. The mean performance scores w.r.t. JS-Divergence and Expected Log Loss, averaged on $r \times s$ sampling distributions, are summarized in Tables 2, 3, 4 and 5. In addition to the performance scores, we also give the best value and worst value w.r.t. the two evaluation criteria. Finally, the overall performance of each algorithm, averaged over all synthesized and all real-world datasets, are shown in Table 6 and Table 7 respectively.

When $k = 0.2 \times m$, in experimental results on synthesized datasets, all TEBC Maxents outperform comparative Maxents in most cases. From Table 6 we can observe that, on average, F-ML-TEBC and B-ML-TEBC are the best two models among TEBC Maxents. The superiority of TEBC Maxents is clearly shown in Tables 2 and 6, under the JS-divergence measure. This superiority also holds under expected log loss measure, which is demonstrated in Tables 3 and 7. As for real-world datasets, we can still draw the same conclusion that TEBC Maxents show their advantages over the others from Tables 4 and 7. Like the results on synthesized datasets, F-ML-TEBC and B-ML-TEBC still show their robustness and become the best two models in the average sense from Tables 6 and 7.

When $k = 0.05 \times m$, the amount of prior information is actually reduced. In this case, it is also clearly demonstrated that all TEBC Maxents outperform comparative Maxents on average. Particularly, we can observe that F-$l_2^2$-TEBC and B-$l_2^2$-TEBC become the most stable and effective, somewhat differing from their performance in the case where $k = 0.2 \times m$.

We would like to mention that in our experiments, standard Maxent and $l_1$-PLUMMET did not perform well. In many cases, using the sampling distribution directly (denoted as Sample) can outperform these two Maxents, especially in the experiment with real-world datasets. One of the causes is that when we fix a unified
\( \delta \) to all the uncertain constraints, it is often in a dilemma: If a small \( \delta \) is used, the feasible region might be far from the underlying real distribution, and hence the optimization procedure can only converge to a poor solution; If a large \( \delta \) is used, there might be a great chance to underfit the sample. Compared with standard Maxent and \( L_1\)-PLUMMET, \( L_1\)-SUMMET (using the selective-update strategy) is relatively stable. However, \( L_1\)-SUMMET with any unified \( \delta \) can not perform as well as TEBC Maxents. Note that there is no practical guidance to determine different \( \delta \) for different uncertain constraints. Even though this guidance exists, it is often a prohibitively-complicated task to find the optimal \( \delta \) for each uncertain constraint. This indeed reflects the implementation complexity of the existing Maxents and highlights the advantage of the parameter-free characteristic of TEBC Maxents. The idea is also supported by the experiment result of SEB Maxents, which achieve better performance than SME and GME on average although are still less effective than TEBCs.

| Method       | Data          | \( U(0, 1) \) | \( |N(0, 1^2)| \) | \( N(3, 1^2) \) |
|--------------|---------------|---------------|----------------|----------------|
| Sample       |               | 0.5983/0.8088 | 0.7005/0.8838  | 0.0000/0.0000  |
| F-JSD-TEBC   |               | 0.8639/0.9572 | 0.8695/0.9966  | 0.9743/1.0000  |
| F-ML-TEBC    | \( 1.0000/1.0000 \) | 0.9985/0.9999 | 0.9983/0.9992  | 0.9919/0.9863  |
| F-JSD-TEBC   |               | 0.8633/0.9571 | 0.8690/0.9962  | 0.9759/0.9955  |
| F-ML-TEBC    |               | 0.9992/0.9994 | 0.9997/0.9997  | 0.9955/0.9879  |
| SME          |               | 0.0000/0.0022 | 0.0231/0.0660  | 0.3774/0.6114  |
| \( L_1\)-SUMMET |               | 0.0017/0.0000 | 0.0000/0.0000  | 0.6376/0.6428  |
| \( L_1\)-PLUMMET |               | 0.0733/0.0356 | 0.0901/0.0577  | 0.4280/0.6269  |
| \( L_2\)-SEB  |               | 0.8392/0.7936 | 0.7190/0.8508  | 0.3398/0.0889  |
| JSD-SEB      |               | 0.9985/0.8494 | 0.9399/0.9296  | 0.3867/0.1172  |
| ML-SEB       |               | 0.8410/0.8496 | 0.9332/0.9299  | 0.3921/0.1176  |
| Best JS Value|               | 0.0120/0.0143 | 0.0133/0.0156  | 0.0091/0.0113  |
| Worst JS Value|              | 0.0262/0.0338 | 0.0281/0.0340  | 0.0182/0.0190  |

| Method       | Data          | \( \chi^2(10) \) | \( \beta(3, 6) \) | \( B(30, 0.2) \) |
|--------------|---------------|-----------------|-----------------|-----------------|
| Sample       |               | 0.0000/0.0000  | 0.0000/0.0000   | 0.0000/0.0000   |
| F-JSD-TEBC   |               | 1.0000/1.0000  | 1.0000/1.0000   | 1.0000/1.0000   |
| F-ML-TEBC    |               | 0.5736/0.7449  | 0.9243/0.8088   | 0.9437/0.8759   |
| F-JSD-TEBC   |               | 0.8830/0.7560  | 0.9347/0.8190   | 0.9534/0.8859   |
| F-ML-TEBC    |               | 0.9963/0.9955  | 0.9967/0.9958   | 0.9957/0.9957   |
| F-JSD-TEBC   |               | 0.8744/0.7409  | 0.9243/0.8040   | 0.9306/0.8709   |
| F-ML-TEBC    |               | 0.8798/0.7518  | 0.9314/0.8147   | 0.9456/0.8807   |
| SME          |               | 0.1469/0.7368  | 0.3995/0.5139   | 0.4686/0.7000   |
| \( L_1\)-SUMMET |               | 0.5311/0.7649  | 0.4859/0.5135   | 0.5623/0.7070   |
| \( L_1\)-PLUMMET |               | 0.3620/0.8002  | 0.3635/0.0790   | 0.3299/0.0954   |
| JSD-SEB      |               | 0.4414/0.1370  | 0.4634/0.1414   | 0.3636/0.1217   |
| ML-SEB       |               | 0.4450/0.1373  | 0.4674/0.1419   | 0.3689/0.1218   |
| Best JS Value|               | 0.0019/0.0128  | 0.0111/0.0129   | 0.0099/0.0113   |
| Worst JS Value|              | 0.0186/0.0190  | 0.0184/0.0189   | 0.0191/0.0184   |

**Table 2** Performance Score (w.r.t. JS-divergence) of different Maxents on Synthesized Datasets
| Method      | Data   | $U(0,1)$ | $|N(0,1^2)|$ | $N(3,1^2)$ |
|------------|--------|----------|----------------|----------|
| Sample     | 0.8599/0.7594 | 0.9119/0.8291 | 0.3802/0.0544 |
| F-JSD-TEBC | 0.9361/0.7871 | 0.9168/1.0000 | 1.0000/1.0000 |
| F-JSD-TEBC | 0.9989/0.9887 | 0.9990/0.9840 | 0.9914/0.9374 |
| F-ML-TEBC  | 1.0000/1.0000 | 1.0000/0.9856 | 0.9982/0.9471 |
| B-JSD-TEBC | 0.9293/0.9863 | 0.9191/0.9993 | 0.9977/0.9958 |
| B-JSD-TEBC | 0.9996/0.9989 | 0.9998/0.9851 | 0.9959/0.9413 |
| SME        | 0.0000/0.1223 | 0.0000/0.0115 | 0.0000/0.0000 |
| $L_1$-SUMMET | 0.7169/0.0919 | 0.7764/0.0000 | 0.8133/0.1741 |
| $L_1$-PLUMMET | 0.5828/0.0000 | 0.6521/0.0192 | 0.5717/0.7539 |
| $L_2$-SEB   | 0.7553/0.5448 | 0.7945/0.4707 | 0.5639/0.0400 |
| JSD-SEB    | 0.9419/0.7853 | 0.9741/0.8590 | 0.6117/0.1514 |
| ML-SEB     | 0.9327/0.7855 | 0.9749/0.8594 | 0.6152/0.1518 |
| Best ELL Value | 6.4128/6.4179 | 6.2935/6.3022 | 6.5928/6.6009 |
| Worst ELL Value | 6.5864/6.4879 | 6.5226/6.3587 | 6.6584/6.6394 |

| Method      | Data   | $\chi^2(10)$ | $\beta(3,6)$ | $B(30,0.2)$ |
|------------|--------|----------------|----------------|--------------|
| Sample     | 0.4724/0.0936 | 0.6084/0.0911 | 0.7054/0.0236 |
| F-JSD-TEBC | 1.0000/1.0000 | 1.0000/1.0000 | 1.0000/1.0000 |
| F-JSD-TEBC | 0.9289/0.7209 | 0.9642/0.7823 | 0.9270/0.8411 |
| F-ML-TEBC  | 0.9298/0.7408 | 0.9693/0.7930 | 0.9803/0.8529 |
| B-JSD-TEBC | 0.9985/0.9967 | 0.9982/0.9962 | 0.9988/0.9959 |
| B-JSD-TEBC | 0.9221/0.7626 | 0.9629/0.7784 | 0.9755/0.8360 |
| B-ML-TEBC  | 0.9279/0.7369 | 0.9679/0.7889 | 0.9788/0.8477 |
| SME        | 0.0000/0.0000 | 0.0000/0.0000 | 0.0000/0.0000 |
| $L_1$-SUMMET | 0.9084/0.8848 | 0.8585/0.9994 | 0.9074/0.7947 |
| $L_1$-PLUMMET | 0.6529/0.8531 | 0.7555/0.7008 | 0.8527/0.7925 |
| $L_2$-SEB   | 0.5335/0.0147 | 0.6291/0.0000 | 0.7546/0.0000 |
| JSD-SEB    | 0.6897/0.1989 | 0.7776/0.1984 | 0.8075/0.1278 |
| ML-SEB     | 0.6918/0.1990 | 0.7793/0.1989 | 0.8085/0.1279 |
| Best ELL Value | 6.5469/6.5531 | 6.5405/6.5491 | 6.5916/6.5834 |
| Worst ELL Value | 6.6129/6.5873 | 6.6267/6.5820 | 6.7347/6.6178 |

Table 3: Performance Scores (w.r.t. Expected Log Loss) of different Maxents on Synthesized Datasets

In summary, TEBC Maxents show their effectiveness and stability, as demonstrated in result tables, especially in Tables 6 and 7. We would like to stress that TEBC Maxents are also easy to implement since only certain constraints and a single TEB constraint are involved. This can help to demonstrate our previous theoretical justification on TEB. In addition, note that the performance of SEB-based models can consistently outperform SME, $L_1$-SUMMET and $L_1$-PLUMMET, though the SEB correction is indeed not exact. This observation indicates that the framework of our generalized Maxent proposed in Section 4.2 has gains in itself.

6.3 TEB-Lidstone vs. Comparative Lidstone and Good-Turing Estimators

When the reliable prior information is not available, Lidstone and Good-Turing estimators are often used in many applications since they are often effective enough, and
| Method       | Data   | Dexter     | Statlog    | ISOLET     | Sonar     |
|--------------|--------|------------|------------|------------|-----------|
| Sample       |        | 0.3852/0.4350 | 0.8212/0.8968 | 0.5107/0.5695 | 0.3325/0.3176 |
| F-JSD-TEBC   |        | 0.9415/1.0000 | 0.8093/0.9010 | 0.8261/0.9997 | 0.9513/1.0000 |
| F-ML-TEBC    |        | 1.0000/0.7634 | 1.0000/1.0000 | 1.0000/0.9598 | 1.0000/0.8328 |
| B-JSD-TEBC   |        | 0.9395/0.9883 | 0.7989/0.9068 | 0.5250/1.0000 | 0.9476/0.9948 |
| B-ML-TEBC    |        | 0.9966/0.9566 | 0.9966/0.9566 | 0.9956/0.8274 | 0.9942/0.8239 |
| SME          |        | 0.9996/0.7624 | 1.0000/0.9999 | 0.9984/0.9582 | 0.9984/0.8289 |
| I1-SUMMET    |        | 0.9394/0.9950 | 0.2099/0.0000 | 0.1384/0.0000 | 0.9953/0.9595 |
| I2-SEB       |        | 0.9531/0.4094 | 0.7533/0.7945 | 0.5821/0.5497 | 0.5665/0.3684 |
| JSD-SEB      |        | 0.8874/0.5702 | 0.9853/0.9716 | 0.8675/0.6704 | 0.8177/0.5095 |
| Best JS Value|        | 0.0144/0.0152 | 0.0132/0.0148 | 0.0132/0.0145 | 0.0134/0.0142 |
| Worst JS Value|       | 0.0213/0.0213 | 0.0337/0.0304 | 0.0227/0.0228 | 0.0201/0.0197 |

results w.r.t certain constraints number $k = 0.2 \times m(left)$ and $0.05 \times m(right)$

Table 4 Performance Score (w.r.t. JS-divergence) of different Maxents on Real-world Datasets

| Method       | Data   | Dexter     | Statlog    | ISOLET     | Sonar     |
|--------------|--------|------------|------------|------------|-----------|
| Sample       |        | 0.9825/0.4710 | 0.9811/0.9884 | 0.9860/0.4702 | 0.9806/0.9648 |
| F-JSD-TEBC   |        | 0.9463/1.0000 | 0.9351/0.9572 | 0.9821/0.9833 | 0.9838/1.0000 |
| F-ML-TEBC    |        | 0.9996/0.7678 | 0.9996/0.9999 | 0.9860/0.9974 | 0.9997/0.9954 |
| B-JSD-TEBC   |        | 1.0000/0.7714 | 1.0000/1.0000 | 1.0000/1.0000 | 1.0000/1.0000 |
| B-ML-TEBC    |        | 0.9999/0.7674 | 0.9998/0.9999 | 0.9887/0.9963 | 0.9996/0.9952 |
| SME          |        | 0.0000/0.5313 | 0.5737/0.4980 | 0.0000/0.5079 | 0.7454/0.5920 |
| I1-SUMMET    |        | 0.9470/0.4908 | 0.8644/0.6724 | 0.8252/0.4840 | 0.8715/0.8095 |
| I2-PLUMMET   |        | 0.8330/0.3286 | 0.0000/0.0000 | 0.6469/0.0000 | 0.0000/0.0000 |
| JSD-SEB      |        | 0.8748/0.4300 | 0.9328/0.8834 | 0.7169/0.5678 | 0.9333/0.9203 |
| Best ELL Value|       | 6.3275/6.3600 | 5.0336/5.0862 | 6.0809/6.2262 | 4.6626/4.6838 |
| Worst ELL Value|      | 6.5260/6.9188 | 5.7561/5.4920 | 6.2318/6.2896 | 5.3435/5.1230 |

results w.r.t certain constraints number $k = 0.2 \times m(left)$ and $0.05 \times m(right)$

Table 5 Performance Scores (w.r.t. Expected Log Loss) of different Maxents on Real-world Datasets

more efficient than Maxent. This set of experiments is constructed to verify the advantage of TEB-Lidstone (F-Lidstone and B-Lidstone) over the involved Lidstone and Good-Turing estimators.

6.3.1 Lidstone and Good-Turing Estimators

In this subsection, we evaluate the effectiveness of F-Lidstone and B-Lidstone estimators which have been described in Section 4.3. Various other Lidstone models, i.e., Laplace estimator (Laplace) and Expected Likelihood Estimator (ELE), serve as comparative algorithms. Motivated by TEB-Lidstone, we also derive a Lidstone estimator from SEB in a similar way to TEB-Lidstone. To identify the rate of probability cor-
Table 6: Overall Performance Score evaluated by JS-Divergence for Experiment Results in Section 6.2

| Algorithms | Synthesized | Real-world | Average    |
|------------|-------------|------------|------------|
| Sample     | 0.2164/0.2821 | 0.5123/0.7762 | 0.3644/0.4837 |
| F-JSD-TEBC | 0.9521/0.9923 | 0.3644/0.4184 | 0.9159/0.9587 |
| F-ML-TEBC  | 0.9618/0.9969 | 0.9999/0.8889 | 0.9809/0.8990 |
| B-JSD-TEBC | 0.9495/0.9893 | 0.8797/0.9935 | 0.9472/0.9818 |
| B-ML-TEBC  | 0.9590/0.9957 | 0.9991/0.8874 | 0.9791/0.9065 |
| SME        | 0.2859/0.4598 | 0.7900/0.6547 | 0.4129/0.2528 |
| I₁-SUMMET | 0.3634/0.4549 | 0.1640/0.1127 | 0.2637/0.2838 |
| I₂-SEB     | 0.6568/0.3313 | 0.6068/0.5305 | 0.5363/0.4399 |
| JSD-SEB    | 0.5712/0.3828 | 0.8879/0.6804 | 0.7296/0.6316 |
| B-JSD-TEBC | 0.9753/0.9978 | 0.9966/0.9009 | 0.9787/0.9042 |
| B-ML-TEBC  | 0.9758/0.9893 | 0.9990/0.9010 | 0.9824/0.9025 |
| SME        | 0.8060/0.2600 | 0.3298/0.3523 | 0.1649/0.1097 |
| I₁-SUMMET | 0.2500/0.4545 | 0.8770/0.6142 | 0.3300/0.2773 |
| I₂-SEB     | 0.6706/0.3830 | 0.8905/0.6807 | 0.7426/0.5319 |
| JSD-SEB    | 0.5712/0.3828 | 0.8879/0.6804 | 0.7296/0.6316 |

Table 7: Overall Performance Score evaluated by Expected Log Loss for Experiment Results in Section 6.2

| Algorithms | Synthesized | Real-world | Average    |
|------------|-------------|------------|------------|
| Sample     | 0.6564/0.3086 | 0.9302/0.7986 | 0.7933/0.5536 |
| F-JSD-TEBC | 0.9753/0.9978 | 0.9966/0.9009 | 0.9787/0.9042 |
| F-ML-TEBC  | 0.9758/0.9893 | 0.9990/0.9010 | 0.9824/0.9025 |
| B-JSD-TEBC | 0.9753/0.9978 | 0.9966/0.9009 | 0.9787/0.9042 |
| B-ML-TEBC  | 0.9758/0.9893 | 0.9990/0.9010 | 0.9824/0.9025 |
| SME        | 0.7989/0.9950 | 0.6068/0.5305 | 0.7933/0.5536 |
| I₁-SUMMET | 0.6706/0.3830 | 0.8905/0.6807 | 0.7426/0.5319 |
| I₂-SEB     | 0.6618/0.1783 | 0.8345/0.5929 | 0.7481/0.3856 |
| JSD-SEB    | 0.7989/0.3868 | 0.7971/0.3845 | 0.8889/0.6106 |
| ML-SEB     | 0.8004/0.3871 | 0.9796/0.8347 | 0.8900/0.6109 |

In addition, some Good-Turing estimators, i.e., the simplest Good-Turing estimator (SimplestGT), Simple Good-Turing (SGT) [Gale and Sampson, 1995] and a low complexity diminishing attenuation estimator (LC-DAE) with some asymptotic guarantee of performance [Orlitsky et al., 2003], are also involved in comparative experiments. Because Good-Turing estimators do not assume the bin number m is given, they only assign a probability sum to all the zero bins w.r.t the sample. In our case in which m is provided, the sum is uniformly distributed to all these zero bins.
6.3.2 Results

We employ the same parameter setting in Table 1 but ignore the parameters in constraints of Maxent, and then run F-Lidstone and B-Lidstone estimators as well as the involved comparative models on the synthesized and real-world datasets. The mean performance scores w.r.t. JS-Divergence and Expected Log Loss over generating times $r$ and sampling times $s$ for each dataset are summarized in Table 8 to Table 11. The overall performance of each algorithm on synthesized and real-world datasets is also demonstrated in Table 12 and Table 13.

| Method         | Data                | $U(0, 1)$ | $|N(0, 1^2)|$ | $N(3, 1^2)$ | $\chi^2(10)$ | $\beta(3, 6)$ | $B(30, 0.2)$ |
|----------------|---------------------|-----------|---------------|-------------|--------------|--------------|--------------|
| Sample         | 0.0000              | 0.0000    | 0.0000        | 0.0000      | 0.0000       | 0.0000       |
| SimplestGT     | 0.1475              | 0.2419    | 0.9228        | 0.0748      | 0.1074       | 0.0423       |
| Laplace        | 0.9042              | 0.2158    | 0.0362        | 0.6732      | 0.6715       | 0.5313       |
| ELE            | 0.5798              | 0.6886    | 0.2860        | 0.3967      | 0.3995       | 0.3076       |
| SGT            | 0.3502              | 0.3881    | 0.3864        | 0.3487      | 0.3491       | 0.3817       |
| LC-DAE         | 0.7220              | 0.8798    | 0.8957        | 0.6389      | 0.6385       | 0.4599       |
| B-Lidstone     | 0.9985              | 0.9258    | 0.9957        | 0.9987      | 0.9996       | 0.9956       |
| F-Lidstone     | 1.0000              | 0.9273    | 1.0000        | 1.0000      | 1.0000       | 1.0000       |
| SEB-Lidstone   | 0.7260              | 0.7349    | 0.5865        | 0.6689      | 0.6642       | 0.6071       |

Table 8 Performance Score (w.r.t. JS-divergence) of different Lidstone and Good-Turing Estimators on Synthesized Datasets

In experimental results on synthesized datasets, it can be observed that F-Lidstone and B-Lidstone estimators, especially F-Lidstone, outperform the other models in most cases. Even in the worst case, they are still more effective than most of the other models. Hence, F-Lidstone and B-Lidstone are on average the best performing among all estimators.
For real-world datasets, we can still come to the same conclusion that F-Lidstone and B-Lidstone outperform the others on average. Although Laplace and ELE could achieve the optimal performance on Dexter and Statlog datasets, the effectiveness of F-Lidstone and B-Lidstone is just slightly lower but their performance on the other datasets, especially ISOLET, is much better than that of the other estimators. Further, it can be observed that in some cases the performance scores evaluated by JS-Divergence and Expected Log Loss are not consistent with each other. The phenomenon
Table 13 Overall Performance Score evaluated by Expected Log Loss for Experiment Results in Section 6.3

| Algorithms      | Synthesized | Real-world | Average |
|-----------------|-------------|------------|---------|
| SimplestGT      | 0.1061      | 0.1864     | 0.1462  |
| Laplace         | 0.7128      | 0.9224     | 0.8176  |
| ELE             | 0.4331      | 0.6555     | 0.5693  |
| SGT             | 0.4049      | 0.3879     | 0.3964  |
| LC-DAE          | 0.6025      | 0.7149     | 0.6587  |
| B-Lidstone      | 0.9846      | 0.9557     | 0.9702  |
| F-Lidstone      | **0.9878**  | **0.9583** | **0.9731** |
| SEB-Lidstone    | 0.6629      | 0.7243     | 0.6936  |

is probably due to the incompleteness of these evaluation criteria, which could only partially reflect the similarity between the resulting distribution and the underlying real distribution. In this sense, the more stable the algorithm is in different similarity criteria, the more effective it could be considered to be. F-Lidstone and B-Lidstone are also optimal in this way.

In summary, when Bayesian-TEB and Frequentist-TEB are applied to the Lidstone framework, the resulting B-Lidstone and F-Lidstone estimators could achieve excellent performance in the expected sense, compared with common Lidstone and Good-Turing estimators. Hence, it can be concluded that TEBs do make sense and can benefit the Lidstone framework.

7 Conclusions and Future Work

This paper proposes the closed-form formulae on the expected Tsallis entropy bias (TEB) under Frequentist and Bayesian frameworks. TEBs give the quantities on the difference between the expected Tsallis entropy of sampling distributions and the Tsallis entropy of the underlying real distribution. It is exact in the sense of unbiasedness and consistency, and hence naturally entails a quantitative re-interpretation of the Maxent principle. In other words, TEBs quantitatively give the answer to the question: Why we should choose the distribution with maximum entropy. We further use TEBs in Maxent and Lidstone frameworks, and both of them show promising results on synthesized and real-world datasets.

In using maximum entropy approach for density estimation, a key challenge lies in the dilemma of uncertain constraints selection: Inappropriate choices may easily cause serious overfitting or underfitting problems. To deal with the challenge, a family of TEB Maxents, namely $l_2$-TEBC, JSD-TEBC and ML-TEBC, are proposed in this paper. Instead of using uncertain constraints selected empirically, the proposed models let its Tsallis entropy converge to the underlying real distribution by compensating expected Tsallis entropy bias, while ensure the resulting distribution to resemble the sampling distribution w.r.t. $l_2$ norm, JS-divergence or Maximum Likelihood. Hence, the resulting distributions are optimal in the expected sense, w.r.t. the above three similarity criteria.

The family of TEB Maxents is a natural generalization of standard Maxent. The important difference between TEB Maxents and standard Maxent is that, the constraints of the former can be derived from reliable prior information (certain constraints) or analytical analysis (TEB constraint), while the latter also has to involve
uncertain constraints demanding empirically parametric selection. It turns out that TEB-C Maxents become parameter-free in this sense. Furthermore, the analytically established TEB constraint can be effective to depress overfitting or underfitting, since it can force the resulting distribution to approach the real one by matching their entropies.

In addition to the Maxent framework, we also demonstrate that there is a natural connection between TEB and another widely used estimator, Lidstone estimator. Specifically, TEB can analytically identify the adaptive rate of probability correction in Lidstone framework. As a result, TEB-Lidstone estimators (F-Lidstone and B-Lidstone) have been developed.

In the future, several extra theoretical issues are worth considering. Firstly, the TEB results might be developed in terms of other $q$ indexes of Tsallis entropy. The unbiased and consistent results w.r.t $q = 1$ is of special interests since Tsallis entropy is equivalent to Shannon entropy in this case. It can be expected that these extended results offer more complete criteria to further solve the overfitting and underfitting. For instance, as an extreme case, if we can give $m$ independent Frequentist-TEB results, the possibility of overfitting and underfitting can be, in principle, ruled out and hence a task of $m$-nominal distribution estimation could become determined. However, other numerical procedures should be devised in order to globally solve the resulting model integrating TEB constraints w.r.t. $q \neq 2$, since the new TEB constraints could be non-convex. Secondly, it is also interesting to develop Bayesian-TEB results w.r.t other Bayesian priors. Finally, we have observed that the two criteria of the estimation quality, i.e., JS-divergence and the expected log loss, occasionally give inconsistent evaluation results. Hence, it is helpful to develop more sophisticated metrics to evaluate the performance of density estimation.

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Appendix A. Standard Deviation of $E^{(m)}_{P,n}(T)$

Proposition 3  Given the uniform probability metric over the $P^{(m)}$, the standard deviation of $E^{(m)}_{P,n}(T)$ denoted by $STD^{(m)}_{n}(T)$, then

$$STD^{(m)}_{n}(T) = \frac{2}{\sqrt{(m-1) \cdot (m+2) \cdot (m+3)}} E^{(m)}_{P,n}(T)$$  \hspace{2cm} (26)$$

Proof Combining the definition of standard deviation with the integral operator $L^{(m-1)}$ defined by Formula[7] we have:

$$STD^{(m)}_{n}(T) = \sqrt{\frac{1}{Z^{(m-1)}} L^{(m-1)} \left\{ \left[ E^{(m)}_{P,n}(T) - E^{(m)}_{u}(T) \right]^2 \right\}}$$

which could be further transformed into

$$STD^{(m)}_{n}(T) = \sqrt{\frac{1}{Z^{(m-1)}} \cdot L^{(m-1)} \left\{ \left[ E^{(m)}_{P,n}(T) \right]^2 - \left[ E^{(m)}_{u}(T) \right]^2 \right\}}$$  \hspace{2cm} (27)$$

Recall that $E^{(m)}_{P,n}(T)$ has been re-expressed in Formula[8] and hence it can be verified that

$$\left[ E^{(m)}_{P,n}(T) \right]^2 = \frac{4}{n^2} \left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right)^2$$

Let $U^{(m-1)}$ denote the set of all product terms in $\left( \sum_{i=1}^{m-1} p_i - \sum_{i=1}^{m-1} p_i^2 - \sum_{i=1}^{m-1} \sum_{j=i+1}^{m-1} p_i \cdot p_j \right)^2$. Then the calculation of $\left[ E^{(m)}_{P,n}(T) \right]^2$ is reduced to solve the closed-form $U^{(m-1)}$ w.r.t. integral operator $L^{(m-1)}$.

Due to the symmetry of integral domain, the properties of $L^{(m-1)}$ in Proposition[8] could be generalized as the followings:

(a) $L^{(m-1)}(p_{i}^r) = L^{(m-1)}(p_{j}^r)$, $1 \leq i, j \leq m-1, r \in \{2, 3, 4\}$

(b) $L^{(m-1)}(p_i \cdot p_j^r) = L^{(m-1)}(p_k \cdot p_l^r), 1 \leq i, j, k, l \leq m-1, i \neq j, k \neq l, r \in \{1, 2, 3\}$

(c) $L^{(m-1)}(p_i^r \cdot p_j^s) = L^{(m-1)}(p_k^r \cdot p_l^s), 1 \leq i, j \leq m-1, i \neq j, k \neq l$

(d) $L^{(m-1)}(p_i \cdot p_j^r \cdot p_k^s) = L^{(m-1)}(p_u \cdot p_v \cdot p_w), 1 \leq i, j, k, u, v, w \leq m-1, i \neq j \neq k, u \neq v \neq w, r, s \in \{2, 3\}$

(e) $L^{(m-1)}(p_i \cdot p_j^r \cdot p_k \cdot p_l^s) = L^{(m-1)}(p_u \cdot p_v \cdot p_w \cdot p_x), 1 \leq i, j, k, l, u, v, w, x \leq m-1, i \neq j \neq k \neq l, u \neq v \neq w \neq x$

Based on the above properties, we can obtain a partition of $U^{(m-1)}$: First, we partition $U^{(m-1)}$ into five different sets subject to the formal constraints of (a)-(e); Second, we further partition each set into subsets subject to different $r$ values (if $r$ is involved in the formal definition of a set). After the above two steps of decomposition, the final partition includes 10 parts and could be represented as below:

Partition $U^{(m)} = \{ \{p_i^2\}, \{p_i^3\}, \{p_i^4\}, \{p_i p_j\}, \{p_i p_j^2\}, \{p_i p_j^3\}, \{p_i p_j^2 p_k\}, \{p_i p_j p_k^2\}, \{p_i p_j p_k p_l\} \}$.

It can checked that the terms in each part give the same result with respect the integral operator $L^{(m-1)}$.

Therefore, if the general term formula of each part and their term numbers could be worked out, the general term formula of $\left[ E^{(m)}_{P,n}(T) \right]^2$ follows directly.
The following equations could be checked:

\[ L^{(m-1)}(p_i^2) = \frac{2!}{(m+1)!} \]
\[ L^{(m-1)}(p_i^3) = \frac{3!}{(m+2)!} \]
\[ L^{(m-1)}(p_i^4) = \frac{3!}{(m+3)!} \]
\[ L^{(m-1)}(p_i \cdot p_j) = \frac{1}{(m+1)!} \]
\[ L^{(m-1)}(p_i \cdot p_j^2) = \frac{2!}{(m+2)!} \]
\[ L^{(m-1)}(p_i \cdot p_j^3) = \frac{3!}{(m+3)!} \]
\[ L^{(m-1)}(p_i^2 \cdot p_j^2) = \frac{4}{(m+3)!} \]
\[ L^{(m-1)}(p_i \cdot p_j \cdot p_k) = \frac{1}{(m+2)!} \]
\[ L^{(m-1)}(p_i \cdot p_j \cdot p_k^2) = \frac{2!}{(m+3)!} \]
\[ L^{(m-1)}(p_i \cdot p_j \cdot p_k \cdot p_i) = \frac{1}{(m+3)!} \]

In addition, the general term formula \( N^{(m-1)}() \) of the term number in each part is given by

\[ N^{(m-1)}(p_i^2) = m - 1 \]
\[ N^{(m-1)}(p_i^3) = -2(m - 1) \]
\[ N^{(m-1)}(p_i^4) = m - 1 \]
\[ N^{(m-1)}(p_i \cdot p_j) = (m - 1)(m - 2) \]
\[ N^{(m-1)}(p_i \cdot p_j^2) = -4(m - 1)(m - 2) \]
\[ N^{(m-1)}(p_i \cdot p_j^3) = 2(m - 1)(m - 2) \]
\[ N^{(m-1)}(p_i^2 \cdot p_j^2) = \frac{3 \cdot (m - 1)(m - 2)}{2} \]
\[ N^{(m-1)}(p_i \cdot p_j \cdot p_k) = -(m - 1)(m - 2)(m - 3) \]
\[ N^{(m-1)}(p_i \cdot p_j \cdot p_k^2) = 2(m - 1)(m - 2)(m - 3) \]
\[ N^{(m-1)}(p_i \cdot p_j \cdot p_k \cdot p_i) = \frac{(m - 1)(m - 2)(m - 3)(m - 4)}{4} \]

Replace \( \left[ E_{P,n}^{(m)}(T) \right]^2 \) by the two sets of general term formulae, and we can get

\[
\frac{1}{Z^{(m-1)}} \cdot L^{(m-1)} \left( \left[ E_{P,n}^{(m)}(T) \right]^2 \right) = \frac{1}{Z^{(m)}} \cdot \frac{4(n - 1)^2}{n^2} \sum_{\alpha \in \text{Partition}[\ell^{(m)}]} L^{(m-1)}(\alpha) \cdot N^{(m-1)}(\alpha)
\]

(28)

Substitute Formula 28 into Formula 27, and then the following equation holds:

\[
\text{STD}_{n}^{(m)}(T) = \frac{n - 1}{n} \sqrt{\frac{(m^3 + 2m^2 - 5m + 2)}{(m + 1)(m + 2)(m + 3)} - \frac{(m - 1)^2}{(m + 1)^2}}
\]
After the simplification, we obtain:
\[
STD_n^m(T) = \frac{2}{\sqrt{(m-1) \cdot (m+2) \cdot (m+3)}} \frac{(n-1)(m-1)}{n(m+1)}
\]

Recall that \(E_n^m(T) = \frac{(n-1)(m-1)}{n(m+1)}\), and hence Formula 28 is proved.

It is clear that, if \(n \approx m\), \(STD_n^m(T) \approx \frac{2}{\sqrt{n(m+1)}} \frac{m-1}{n(m+1)}\). Recall that \(\frac{m-1}{n(m+1)}\) is uniform Bayesian-TEB. Hence, the estimation of uniform Bayesian-TEB is relatively stable in the case of inadequate sampling.

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