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ESTIMATION OF ENTROPIES AND DIVERGENCES VIA NEAREST NEIGHBORS

NIKOLAI LEONENKO — LUC PRONZATO — VIPPAL SAVANI

ABSTRACT. We extend the results in [L. F. Kozachenko, N. N. Leonenko: *On statistical estimation of entropy of random vector*, Problems Inform. Transmission **23** (1987), 95–101; Translated from Problemy Peredachi Informatsii 23 (1987), 9–16 (in Russian)] and [M. N. Goria, N. N. Leonenko, V. V. Mergel, P. L. Novi Inverardi: *A new class of random vector entropy estimators and its applications in testing statistical hypotheses*, J. Nonparametr. Statist. **17** (2005), 277–297] and show how k th nearest-neighbor distances in a sample of N i.i.d. vectors distributed with the probability density f can be used to estimate consistently Rényi and Tsallis entropies of the unknown f under minimal assumptions. The method is extended to the estimation of statistical distances between two distributions in the case when one i.i.d. sample from each is available.

1. Introduction

Let $X \in \mathbb{R}^m$ be a random vector with probability measure μ having the density f with respect to the Lebesgue measure $\mu_{\mathcal{L}}$. The Rényi entropy [24] of f is defined by

$$H_q^* = \frac{1}{1-q} \log \int_{\mathbb{R}^m} f^q(x) dx, \quad q \neq 1, \quad (1)$$

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and the Havrda—Charvát entropy [8] (also called Tsallis entropy [25]) by

$$H_q = \frac{1}{q-1} \left(1 - \int_{\mathbb{R}^m} f^q(x) dx \right), \quad q \neq 1. \tag{2}$$

When q tends to 1, both H_q and H_q^* tend to the Shannon entropy

$$H_1 = - \int_{\mathbb{R}^m} f(x) \log f(x) dx. \tag{3}$$

We consider the estimation of H_q^* and H_q from a sample of N independent and identically distributed (i.i.d.) random variables X_1, \dots, X_N , $N \geq 2$, extending the approach proposed by Kozachenko and Leonenko, see [12], [7], for the estimation of H_1 . The method is based on nearest-neighbor distances in the sample (when $m = 1$, it is thus related to sample-spacing methods; see, e.g., [29] for Shannon entropy and [2] for a survey on entropy estimation). It is connected with the random-graph approach of Redmond and Yurich [23] who, supposing that the distribution is supported on $[0, 1]^m$ and with some smoothness assumptions on f , construct a strongly consistent estimator of H_q^* for $0 < q < 1$ (up to an unknown bias term independent of f , related to the graph properties). For $q \neq 1$ our construction relies on the estimation of the integral

$$I_q = I_q(f) = \mathbb{E}\{f^{q-1}(X)\} = \int_{\mathbb{R}^m} f^q(x) dx \tag{4}$$

through the computation of conditional moments of nearest-neighbor distances (\mathbb{E} will always denote the expectation for f). It thus possesses some similarities with [6] where the asymptotic behavior of the moments of k th nearest-neighbor distances is considered: under the conditions that f is continuous, $f > 0$ on a compact convex subset \mathcal{C} of \mathbb{R}^m , with f having bounded partial derivatives on \mathcal{C} , the weak consistency of the estimator of I_q is established, $N \rightarrow \infty$, for $m \geq 2$ and $q < 1$. Comparatively, our results cover a larger range of values for q and do not rely on regularity or bounded support assumptions for f . The results for the estimation of the Shannon entropy (3) are derived from those obtained for $q \neq 1$.

The method can also be applied to the estimation of statistical distances. Here we only consider the Kullback-Leibler relative entropy, defined by

$$K(f, g) = \int_{\mathbb{R}^m} f(x) \log \frac{f(x)}{g(x)} dx = \check{H}_1 - H_1, \tag{5}$$

where H_1 is given by (3) and

$$\check{H}_1 = - \int_{\mathbb{R}^m} f(x) \log g(x) dx. \quad (6)$$

The estimation of H_1 and \check{H}_1 is then based on N independent observations X_1, \dots, X_N distributed with the density f and M observations Y_1, \dots, Y_M distributed with g . Estimation of other statistical distances is considered in [14].

Section 2 gives some properties of I_q , H_q^* and H_q and lists some applications of entropy estimation. The main results of the paper are presented in Section 3, where the nearest-neighbor estimators of the quantities (1–5) are defined and their asymptotic properties are summarized.

2. Some properties of I_q , H_q , H_q^* and applications

One may notice that H_q^* can be expressed as a function of H_q , $H_q^* = \log[1 - (q - 1)H_q]/(1 - q)$, with $d(H_q^*)/d(H_q) = 1/I_q$ and $d^2(H_q^*)/d(H_q)^2 = (q - 1)/I_q^2$ for any q . H_q^* is thus a strictly increasing concave (resp. convex) function of H_q for $q < 1$ (resp. $q > 1$). A distribution that maximizes H_q^* therefore also maximizes H_q and will be called q -entropy maximizing. The entropy H_q is a concave (resp. convex) function of the density for $q > 0$ (resp. $q < 0$). Hence, q -entropy maximizing distributions, under some specific constraints, are uniquely defined for $q > 0$. For instance, when the constraint is that the distribution is finitely supported, then the q -entropy maximizing distribution is uniform. Also, for any dimension $m \geq 1$ the q -entropy maximizing distribution with a given covariance matrix is of the multidimensional Student- t type if $m/(m + 2) < q < 1$ and has a finite support if $q > 1$, see [30]. This generalizes the well-known property that Shannon entropy H_1 is maximized for the normal distribution. Such entropy-maximization properties can be used to derive nonparametric statistical tests, following the same approach as in [29] where normality is tested with H_1 ; see also [7]. The q -entropy maximizing property of the Student distribution can be used to test that a given sample is Student distributed, which finds applications in financial mathematics, see [11]. The entropy (2) is of interest in the study of nonlinear Fokker-Planck equations, see [26]. Values of $q \in [1, 3]$ are used in [1] to study the behavior of fractal random walks. Applications for quantizer design, characterization of time-frequency distributions, image registration and indexing, texture classification, image matching etc., are considered in [10], [9], [20]. Entropy minimization is used in [22], [32] for parameter estimation in semi-parametric models. Entropy estimation is a basic tool for independent component analysis in signal processing, see, e.g., [18]. The Kullback-Leibler relative

entropy (5) can be used to construct a measure of mutual information (MI) between statistical distributions, with applications in image [31], [20] and signal processing [18].

3. The estimators and their properties

3.1. The estimators

Suppose that X_1, \dots, X_N , $N \geq 2$, are i.i.d. with a probability measure μ having a density f with respect to the Lebesgue measure. Let $\rho(x, y)$ denote the Euclidean distance between two points x, y of \mathbb{R}^m . For a given sample X_1, \dots, X_N , and a given X_i in the sample, from the $N - 1$ distances $\rho(X_i, X_j)$, $j = 1, \dots, N$, $j \neq i$, we form the order statistics $\rho_{1,N-1}^{(i)} \leq \rho_{2,N-1}^{(i)} \leq \dots \leq \rho_{N-1,N-1}^{(i)}$, so that $\rho_{k,N-1}^{(i)}$ is the k th nearest-neighbor distance from X_i to some other X_j in the sample, $j \neq i$. We estimate I_q (4) for $q \neq 1$, by

$$\hat{I}_{N,k,q} = \frac{1}{N} \sum_{i=1}^N (\zeta_{N,i,k})^{1-q}, \tag{7}$$

with $\zeta_{N,i,k} = (N - 1) C_k V_m (\rho_{k,N-1}^{(i)})^m$, where $V_m = \pi^{m/2} / \Gamma(m/2 + 1)$ is the volume of the unit ball $\mathcal{B}(0, 1)$ in \mathbb{R}^m and $C_k = [\Gamma(k) / \Gamma(k + 1 - q)]^{1/(1-q)}$. Then we estimate H_q^* (1) and H_q (2) respectively by

$$\hat{H}_{N,k,q}^* = \log(\hat{I}_{N,k,q}) / (1 - q), \tag{8}$$

$$\hat{H}_{N,k,q} = (1 - \hat{I}_{N,k,q}) / (q - 1). \tag{9}$$

For the estimation of H_1 (3) we take the limit of $\hat{H}_{N,k,q}$ as $q \rightarrow 1$, which gives

$$\hat{H}_{N,k,1} = \frac{1}{N} \sum_{i=1}^N \log \xi_{N,i,k} \tag{10}$$

with $\xi_{N,i,k} = (N - 1) \exp[-\Psi(k)] V_m (\rho_{k,N-1}^{(i)})^m$, where $\Psi(z) = \Gamma'(z) / \Gamma(z)$ is the digamma function.

Suppose now that X_1, \dots, X_N are i.i.d. with the density f and that Y_1, \dots, Y_M are i.i.d. with the density g . For any X_i in the sample, $i \in \{1, \dots, N\}$, consider $\check{\rho}(X_i, Y_j)$, $j = 1, \dots, M$, and form the order statistics $\check{\rho}_{1,M}^{(i)} \leq \check{\rho}_{2,M}^{(i)} \leq \dots \leq \check{\rho}_{M,M}^{(i)}$, so that $\check{\rho}_{k,M}^{(i)}$ is the k th nearest-neighbor distance from X_i to some Y_j ,

$j \in \{1, \dots, M\}$. Then we estimate \check{H}_1 (6) and $K(f, g)$ (5) respectively by

$$\check{H}_{N,M,k} = \frac{1}{N} \sum_{i=1}^N \log \left\{ M \exp[-\Psi(k)] V_m \left(\check{\rho}_{k,M}^{(i)} \right)^m \right\}, \tag{11}$$

$$\hat{K}_{N,M,k} = \check{H}_{N,M,k} - \hat{H}_{N,k,1} = m \log \left[\prod_{i=1}^N \frac{\check{\rho}_{k,M}^{(i)}}{\rho_{k,N}^{(i)}} \right]^{1/N} + \log \frac{M}{N-1}. \tag{12}$$

3.2. Asymptotic properties

The properties of the estimators $\hat{I}_{N,k,q}$ (7) are summarized in Table 1, from which one can deduce those of $\hat{H}_{N,k,q}^*$ (8) and $\hat{H}_{N,k,q}$ (9). Table 2 gives the properties of the estimators $\hat{H}_{N,k,1}$ (10) and $\check{H}_{N,M,k}$ (11), from which those of the estimator $\hat{K}_{N,M,k}$ (12) can be read directly. As indicated, L_2 (and thus weak) consistency is obtained without any smoothness assumption on the underlying density f (or densities f and g) or any bounded-support assumption, which improves the results of existing methods, see [2]. The proofs are rather technical and are omitted due to space limitation, see [14]. They rely on an application of Lebesgue’s bounded convergence theorem, on Theorem 2.5.1 of [4], p. 34, on the generalized Helly-Bray Lemma, see [16], p. 187 and on the following.

Lemma 1 (Lebesgue, [13]). If $g \in L_1(\mathbb{R}^m)$, then for any sequence of open balls $\mathcal{B}(x, R_k)$ of radius tending to zero as $k \rightarrow \infty$ and for $\mu_{\mathcal{L}}$ -almost any $x \in \mathbb{R}^m$, $\lim_{k \rightarrow \infty} [1/(V_m R_k^m)] \int_{\mathcal{B}(x, R_k)} g(t) dt = g(x)$.

TABLE 1. Asymptotic properties of the estimator (7) as $N \rightarrow \infty$.

q	assumption on f	$\hat{I}_{N,k,q}$
$q < 1$	$\mathbb{E}\{f^{q-1}(X)\} < \infty$	asympt. unbiased
$q < 1$	$\mathbb{E}\{f^{2(q-1)}(X)\} < \infty$	L_2 -consistent
$1 < q < k + 1$	f bounded	asympt. unbiased
$1 < q < (k + 1)/2$	f bounded, $k \geq 2$	L_2 -consistent
$1 < q < 3/2$	f bounded, $k = 1$	L_2 -consistent

TABLE 2. Asymptotic properties of the estimators (10) and (11).

assumptions on f and g	property
f bounded, $\exists \epsilon > 0: \mathbb{E}\{f^{-\epsilon}(X)\} < \infty$	$\hat{H}_{N,k,1}$ is L_2 -consistent, $N \rightarrow \infty$
g bounded, $\exists \epsilon > 0: \mathbb{E}\{g^{-\epsilon}(X)\} < \infty$	$\check{H}_{N,M,k}$ is L_2 -consistent, $N, M \rightarrow \infty$

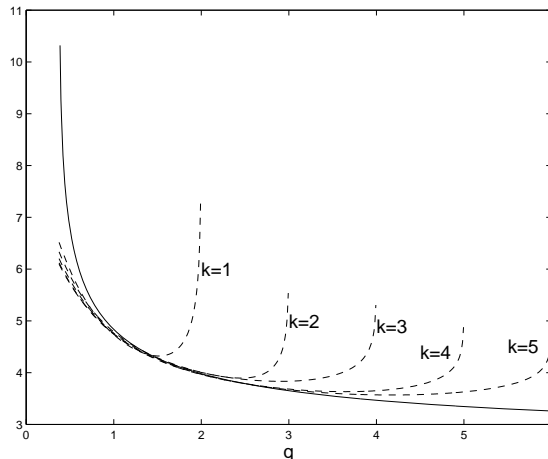


FIGURE 1. H_q^* (solid line) and $\hat{H}_{N,k,q}^*$ (dashed lines) as functions of q for the Student distribution $T(5, \mathbf{I}_3)$ in \mathbb{R}^3 with zero-mean and identity scaling matrix ($N = 1000$).

EXAMPLE. Figure 1 presents H_q^* as a function of q (solid line) for the three-dimensional ($m = 3$) Student distribution $T(\nu, \mathbf{I}_3)$ with zero mean, scaling matrix the identity \mathbf{I}_3 (and covariance matrix $\nu/(\nu - 2)$ times the identity) and $\nu = 5$ degrees of freedom, the p.d.f. of which is

$$f_\nu(x) = \frac{1}{(\nu\pi)^{m/2}} \frac{\Gamma(\frac{m+\nu}{2})}{\Gamma(\frac{\nu}{2})} \frac{1}{[1 + x^\top x/\nu]^{(m+\nu)/2}}, \quad x \in \mathbb{R}^m.$$

The associated Rényi entropy H_q^* is given by

$$H_q^* = \frac{1}{1 - q} \log \frac{B(\frac{q(m+\nu)}{2} - \frac{m}{2}, \frac{m}{2})}{B^q(\frac{\nu}{2}, \frac{m}{2})} + \frac{1}{2} \log[(\pi\nu)^m] - \log \Gamma\left(\frac{m}{2}\right)$$

with $B(u, v) = \Gamma(u)\Gamma(v)/\Gamma(u + v)$ the Beta function, and is defined for $q > m/(m + \nu) = 3/8 = 0.375$. The estimates $\hat{H}_{N,k,q}^*$ for $k = 1, \dots, 5$ obtained from a sample of size $N = 1000$ are plotted on the same figure. Note that $\hat{H}_{N,k,q}^*$ is defined only for $q < k + 1$.

Further developments. Here nearest neighbors are defined for the Euclidean distance, but the metric could be adapted to the observed sample. Indeed, for X_1, \dots, X_N a sample having a non-spherical distribution, its empirical covariance matrix $\hat{\Sigma}_N$ could be used to define a new metric through $\|x\|_{\hat{\Sigma}_N}^2 = x^\top \hat{\Sigma}_N^{-1} x$, the volume V_m of the unit ball in this metric becoming $|\hat{\Sigma}_N|^{1/2} \pi^{m/2} / \Gamma(m/2 + 1)$.

Few results exist concerning \sqrt{N} -consistency of entropy estimators. For instance, \sqrt{N} -consistency of an estimator of H_1 based on nearest-neighbor distances ($k = 1$) is proved in [27] for $m = 1$ and sufficiently regular densities f with unbounded support. Concerning the method proposed here, \sqrt{N} -consistency of the estimator $\hat{I}_{N,k,q}$ is still an open issue. As for the case of spacing methods, where the spacing m can be taken as an increasing function of the sample size N , see, e.g., [29], [28], it seems reasonable to let $k = k_N$ increase with N . Properties of nearest-neighbor distances with $k_N \rightarrow \infty$ are considered for instance in [17], [19], [5], [15].

A central limit theorem for functions $h(\rho)$ of nearest-neighbor distances is obtained in [3] for $k = 1$ and in [21] for $k \geq 1$. However, these results are restricted to the case of bounded functions, which does not cover the situation $h(\rho) = \rho^{m(1-q)}$, see (7), or $h(\rho) = \log(\rho)$, see (10). Conditions for the asymptotic normality of $\hat{I}_{N,k,q}$ are under current investigation.

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