Tatra Mt. Math. Publ. **39** (2008), 265–273

TATRA MOUNTAINS
Mathematical Publications

ESTIMATION OF ENTROPIES AND DIVERGENCES VIA NEAREST NEIGHBORS

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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 kth nearest-neighbor distances in a sample of N i.i.d. vectors distributed with the probability density f can be used to estimate consistently Rény 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

$$H_q^* = \frac{1}{1-q} \log \int_{\mathbb{R}^m} f^q(x)\, \mathrm{d}x\,, \qquad q \neq 1\,, \tag{1}$$

2000 Mathematics Subject Classification: 94A15, 62G20.
Keywords: entropy estimation, estimation of statistical distance, estimation of divergence, nearest-neighbor distances, Rényi entropy, Havrda-Charvát entropy, Tsallis entropy.
The first author gratefully acknowledges financial support from EPSRC grant RCMT 119. The work of the second author was partially supported by the IST Programme of the European Community, under the PASCAL Network of Excellence, IST-2002-506778. This publication only reflects the authors's view.

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

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

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

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

We consider the estimation of H_q^* and H_q from a sample of N independent and identically distributed (i.i.d.) random variables $X_1, \ldots, X_N$, $N \geq 2$, 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 Yukich [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

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

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 kth 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, $N \to \infty$, 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

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

where H_1 is given by (3) and

$$\breve{H}_1 = -\int_{\mathbb{R}^m} f(x)\, \log g(x)\, \mathrm{d}x\,. \tag{6}$$

The estimation of H_1 and $\breve{H}_1$ is then based on N independent observations $X_1, \ldots, X_N$ distributed with the density f and M observations $Y_1, \ldots, Y_M$ 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, $H_q^* = \log\bigl[1 - (q-1)H_q\bigr]/(1-q)$, 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 $\rho^{(i)}_{1,N-1} \leq \rho^{(i)}_{2,N-1} \leq \cdots \leq \rho^{(i)}_{N-1,N-1}$, so that $\rho^{(i)}_{k,N-1}$ is the kth 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 $\zeta_{N,i,k} = (N-1)\, C_k\, V_m \left(\rho^{(i)}_{k,N-1}\right)^m$, 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 $C_k = \left[\Gamma(k)/\Gamma(k+1-q)\right]^{1/(1-q)}$. 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 $q \to 1$, which gives

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

with $\xi_{N,i,k} = (N-1)\, \exp\left[-\Psi(k)\right] V_m \left(\rho^{(i)}_{k,N-1}\right)^m$, 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 $\breve{\rho}(X_i, Y_j)$, $j = 1, \dots, M$, and form the order statistics $\breve{\rho}^{(i)}_{1,M} \leq \breve{\rho}^{(i)}_{2,M} \leq \cdots \leq \breve{\rho}^{(i)}_{M,M}$, so that $\breve{\rho}^{(i)}_{k,M}$ is the kth nearest-neighbor distance from X_i to some Y_j,

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

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

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

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 $\breve{H}_{N,M,k}$ (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 $k \to \infty$ and for $\mu_{\mathcal{L}}$-almost any $x \in \mathbb{R}^m$, $\lim_{k\to\infty} \left[1/(V_m R_k^m)\right] \int_{\mathcal{B}(x,R_k)} g(t)\,\mathrm{d}t = g(x)$.

Table 1. Asymptotic properties of the estimator (7) as $N \to \infty$.

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, $N \to \infty$
g bounded, $\exists \epsilon > 0$: $\mathbb{E}\{g^{-\epsilon}(X)\} < \infty$	$\breve{H}_{N,M,k}$ is L_2-consistent, $N, M \to \infty$

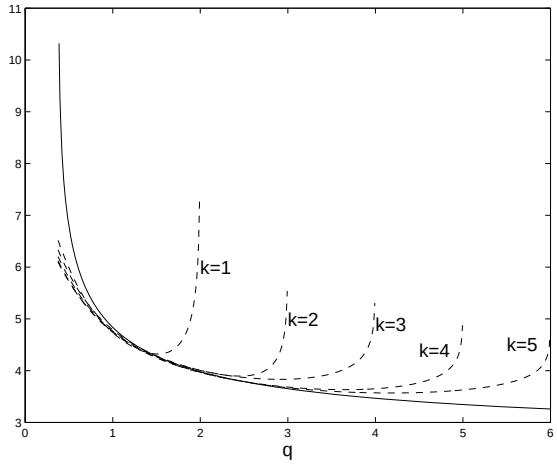

FIGURE 1. H_q^* (solid line) and $\hat{H}_{N,k,q}^*$ (dashed lines) as functions of q for the Student distribution $T(5, \mathbf{I}_3)$ in $\mathbb{R}^3$ with zero-mean and identity scaling matrix ($N = 1000$).

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

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

The associated Rényi entropy H_q^* is given by

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

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 $k = 1, \ldots, 5$ 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 $X_1, \ldots, X_N$ 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 $k_N \to \infty$ 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.

Acknowledgements. The authors wish to thank Anatoly A. Zhigljavsky from Cardiff School of Mathematics for helpful discussions.

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Received September 20, 2006

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