Statistical Inference for Rényi Entropy Functionals

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Abstract

Numerous entropy-type characteristics (functionals) generalizing Rényi entropy are widely used in mathematical statistics, physics, information theory, and signal processing for characterizing uncertainty in probability distributions and distribution identification problems. We consider estimators of some entropy (integral) functionals for discrete and continuous distributions based on the number of epsilon-close vector records in the corresponding independent and identically distributed samples from two distributions. The estimators form a triangular scheme of generalized \textit{U}-statistics. We show the asymptotic properties of these estimators (e.g., consistency and asymptotic normality). The results can be applied in various problems in computer science and mathematical statistics (e.g., approximate matching for random databases, record linkage, image matching).

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1 Introduction

Let \(X\) and \(Y\) be \(d\)-dimensional random vectors with discrete or continuous distributions \(P_X\) and \(P_Y\), respectively. In information theory and statistics, there are various generalizations of Shannon entropy (see Shannon, 1948), characterizing uncertainty in \(P_X\) and \(P_Y\), for example, the Rényi entropy (Rényi, 1961, 1970),

\[
h_s := \frac{1}{1-s} \log \left( \int_{R^d} p_X(x)^s dx \right), \quad s \neq 1,
\]

and the (differentiable) variability for approximate record matching in random databases

\[
v := -\log \left( \int_{R^d} p_X(x)p_Y(x) dx \right),
\]

where \(p_X(x), p_Y(x), x \in R^d\), are densities of \(P_X\) and \(P_Y\), respectively (see Seleznjev and Thalheim, 2003, 2008). Henceforth we use \(\log x\) to denote the natural logarithm of \(x\). More generally, for non-negative integers \(r_1, r_2 \geq 0\) and \(r := (r_1, r_2)\), we consider Rényi entropy functionals

\[
q_r := \int_{R^d} p_X(x)^{r_1}p_Y(x)^{r_2} dx,
\]
and for the discrete case, $\mathcal{P}_X = \{p_X(k), k \in \mathbb{N}^d\}$ and $\mathcal{P}_Y = \{p_Y(k), k \in \mathbb{N}^d\}$,

$$q_r := \sum_k p_X(k)^r p_Y(k)^{r_2},$$

i.e., $q_r = q_{r_1,r_2}$. Then, for example, the Rényi entropy $h_s = h_{s,0} = \log(q_{s,0})/(1-s)$ and the variability $v = h_{1,1} = - \log(q_{1,1})$. Let $X_1,\ldots,X_{n_1}$ and $Y_1,\ldots,Y_{n_2}$ be mutually independent samples of independent and identically distributed (i.i.d.) observations from $\mathcal{P}_X$ and $\mathcal{P}_Y$, respectively. We consider the problem of estimating the entropy-type functionals $q_r$ and related characteristics for $\mathcal{P}_X$ and $\mathcal{P}_Y$ from the samples $X_1,\ldots,X_{n_1}$ and $Y_1,\ldots,Y_{n_2}$.

Various entropy applications in statistics (e.g., classification and distribution identification problems) and in computer science and bioinformatics (e.g., average case analysis for random databases, approximate pattern and image matching) are investigated in, e.g., Kapur (1989), Kapur and Kesavan (1992), Leonenko et al. (2008), Szpankowski (2001), Seleznjev and Thalheim (2003, 2008), Thalheim (2000), Baryshnikov et al. (2009), and Leonenko and Seleznjev (2010). Some average case analysis problems for random databases with entropy characteristics are investigated also in Demetrovics et al. (1995, 1998a, 1998b).

In our paper, we generalize the results and approach proposed in Leonenko and Seleznjev (2010), where the quadratic Rényi entropy estimation is studied for one sample. We consider properties (consistency and asymptotic normality) of kernel-type estimators based on the number of coincident (or $\epsilon$-close) observations in $d$-dimensional samples for more general class of entropy-type functionals. These results can be used, e.g., in evaluating of asymptotical confidence intervals for the corresponding Rényi entropy functionals.

Note that our estimators of entropy-type functionals are different form those considered by Kozachenko and Leonenko (1987), Tsybakov and van der Meulen (1996), Leonenko et al. (2008), and Baryshnikov et al. (2009) (see Leonenko and Seleznjev, 2010, for a discussion).

First we introduce some notation. Throughout the paper, let $X$ and $Y$ be independent random vectors in $\mathbb{R}^d$ with distributions $\mathcal{P}_X$ and $\mathcal{P}_Y$, respectively. For the discrete case, $\mathcal{P}_X = \{p_X(k), k \in \mathbb{N}^d\}$ and $\mathcal{P}_Y = \{p_Y(k), k \in \mathbb{N}^d\}$. In the continuous case, let the distributions be with densities $p_X(x)$ and $p_Y(x)$, $x \in \mathbb{R}^d$, respectively. Let $d(x,y) = |x-y|$ denote the Euclidean distance in $\mathbb{R}^d$ and $B_\epsilon(x) := \{y : d(x,y) \leq \epsilon\}$ an $\epsilon$-ball in $\mathbb{R}^d$ with center at $x$, radius $\epsilon$, and volume $b_\epsilon(d) = \epsilon^d b_1(d)$, $b_1(d) = 2\pi^{d/2}/(d!)$). Denote by $p_{X,\epsilon}(x)$ the $\epsilon$-ball probability

$$p_{X,\epsilon}(x) := P\{X \in B_\epsilon(x)\}.$$ 

We write $I(C)$ for the indicator of an event $C$, and $|D|$ for the cardinality of a finite set $D$.

Next we define the following estimators of $q_r$ when $r_1$ and $r_2$ are non-negative integers. Let the i.i.d. samples $X_1,\ldots,X_{n_1}$ and $Y_1,\ldots,Y_{n_2}$ be from $\mathcal{P}_X$ and $\mathcal{P}_Y$, respectively. Denote $n := (n_1,n_2)$, $n := n_1 + n_2$, and say that $n \to \infty$ if $n_1,n_2 \to \infty$ and let $p_n := n_1/n \to p$, $0 < p < 1$, as $n \to \infty$.

For an integer $k$, denote by $S_{m,k}$ the set of all $k$-subsets of $\{1,\ldots,m\}$. For $S \in S_{n_1,r_1}$, $T \in S_{n_2,r_2}$, and $i \in S$, define

$$\psi_n^{(i)}(S;T) := I(d(X_i, X_j) \leq \epsilon, d(X_i, Y_k) \leq \epsilon, \forall j \in S, \forall k \in T),$$
i.e., the indicator of the event that all elements in \(\{X_j, j \in S\}\) and \(\{Y_k, k \in T\}\) are \(\epsilon\)-close to \(X_i\). Note that by conditioning we have

\[
E\psi_n^{(i)}(S; T) = E p_{X,\epsilon}(X)^{r_1-1} p_{Y,\epsilon}(X)^{r_2} =: q_{r,\epsilon},
\]

say, the \(\epsilon\)-coincidence probability. Let a generalized \(U\)-statistic for the functional \(q_{r,\epsilon}\) be defined as

\[
Q_n = Q_{n,r,\epsilon} := \left(\frac{n_1}{r_1}\right)^{-1} \left(\frac{n_2}{r_2}\right)^{-1} \sum_{(n_1,r_1)} \sum_{(n_2,r_2)} \psi_n(S; T),
\]

where the symmetrized kernel

\[
\psi_n(S; T) := \frac{1}{r_1} \sum_{i \in S} \psi_n^{(i)}(S; T),
\]

and by definition, \(Q_n\) is an unbiased estimator of \(q_{r,\epsilon} = EQ_n\). Define for discrete and continuous distributions

\[
\zeta_{1,0} := \text{Var}(p_X(X)^{r_1-1} p_Y(X)^{r_2}) = q_{2r_1-1,2r_2} - q_{r_1,r_2}^2,
\]

\[
\zeta_{0,1} := \text{Var}(p_X(Y)^{r_1} p_Y(Y)^{r_2-1}) = q_{2r_1,2r_2-1} - q_{r_1,r_2}^2,
\]

\[
\kappa := p^{-1} \zeta_{1,0} + (1-p)^{-1} \zeta_{0,1}.
\]

Let \(\xrightarrow{D}\) and \(\xrightarrow{P}\) denote convergence in distribution and in probability, respectively.

The paper is organized as follows. In Section 2 we consider estimation of Rényi entropy functionals for discrete and continuous distributions. In Section 3 we discuss some applications of the obtained estimators in average case analysis for random databases (e.g., for join optimization with approximate matching), in pattern and image matching problems, and for some distribution identification problems. Several numerical experiments demonstrate the rate of convergence in the obtained asymptotic results. Section 4 contains the proofs of the statements from the previous sections.

## 2 Main Results

### 2.1 Discrete Distributions

In the discrete case, set \(\epsilon = 0\), i.e., exact coincidences are considered. Then \(Q_n\) is an unbiased estimator of the \(\epsilon\)-coincidence probability

\[
q_{r,0} = q_r = EI(X_1 = X_i = Y_j, i = 2, \ldots, r_1, j = 1, \ldots, r_2) = E p_X(X)^{r_1-1} p_Y(X)^{r_2}.
\]

Let \(Q_{n,r} := Q_{n,r,0}\) and

\[
K_n := p_n^{-1} r_1^2 (Q_{n,2r_1-1,2r_2} - Q_{n,r}^2) + (1-p_n)^{-1} r_2^2 (Q_{n,2r_1,2r_2-1} - Q_{n,r}^2),
\]

and \(k_n := \max(K_n, 1/n)\), an estimator of \(\kappa\). Denote by \(H_n := \log(\max(Q_n, 1/n))/(1 - r)\), an estimator of \(h_r := \log(q_r)/(1 - r)\).
Remark. Instead of 1/n in the definition of a truncated estimator, a sequence \( a_n > 0, a_n \to 0 \) as as \( n \to \infty \), can be used (cf. Leonenko and Seleznjev, 2010).

The next asymptotic normality theorem for the estimator \( Q_n \) follows straightforwardly from the general \( U \)-statistic theory (see, e.g., Lee, 1990, Koroljuk and Borovskich, 1994) and the Slutsky theorem.

**Theorem 1** If \( \zeta_{1,0}, \zeta_{0,1} > 0 \), then

\[
\sqrt{n}(Q_n - q_r) \overset{D}{\to} N(0, \kappa) \quad \text{and} \quad \sqrt{n}(Q_n - q_r)/k_n^{1/2} \overset{D}{\to} N(0, 1);
\]

\[
\sqrt{n}(1 - r) Q_n/k_n^{1/2} (H_n - h_r) \overset{D}{\to} N(0, 1) \quad \text{as} \quad n \to \infty.
\]

### 2.2 Continuous Distributions

In the continuous case, denote by \( \tilde{Q}_n := Q_n/b_r(d)^{-1} \) an estimator of \( q_r \). Let \( \tilde{q}_{r,e} := E\tilde{Q}_n = q_{r,e}/b_r(d)^{-1} \) and \( v_n^2 := \text{Var}(\tilde{Q}_n) \).

Henceforth, assume that \( \epsilon = e(n) \to 0 \) as \( n \to \infty \). For a sequence of random variables \( U_n, n \geq 1 \), we say that \( U_n = \text{Op}(1) \) as \( n \to \infty \) if for any \( \epsilon > 0 \) and \( n \) large enough there exists \( A > 0 \) such that \( P(|U_n| > A) \leq \epsilon \), i.e., the family of distributions of \( U_n, n \geq 1 \), is tight, and for a numerical sequence \( w_n, n \geq 1 \), say, \( U_n = \text{Op}(w_n) \) as \( n \to \infty \) if \( U_n/w_n = \text{Op}(1) \) as \( n \to \infty \). The following theorem describes the consistency and asymptotic normality properties of the estimator \( \tilde{Q}_n \).

**Theorem 2** Let \( p_X(x) \) and \( p_Y(x) \) be bounded and continuous or with a finite number of discontinuity points.

(i) \( v_n^2 = O(n^{-1} e^{d(1/r-1)}) \) and \( E\tilde{Q}_n \to q_r \) as \( n \to \infty \), and hence if \( n e^{d(1-1/r)} \to \infty \) as \( n \to \infty \), then \( \tilde{Q}_n \) is a consistent estimator of \( q_r \).

(ii) If \( n e^{d} \to \infty \) as \( n \to \infty \) and \( \zeta_{1,0}, \zeta_{0,1} > 0 \), then

\[
\sqrt{n}(\tilde{Q}_n - \tilde{q}_{r,e}) \overset{D}{\to} N(0, \kappa) \quad \text{as} \quad n \to \infty.
\]

In order to evaluate the functional \( q_r \), we denote by \( H^{(\alpha)}(C), 0 < \alpha \leq 2, C > 0 \), a linear space of bounded and continuous in \( R^d \) functions satisfying \( \alpha \)-Hölder condition if \( 0 < \alpha \leq 1 \) or if \( 1 < \alpha \leq 2 \) with continuous partial derivatives satisfying \( (\alpha - 1)\)-Hölder condition with constant \( C \). Furthermore, let

\[
K_n := p_n^{-1}r_1^2(\tilde{Q}_{n,2r_1-1,2r_2,e} - \tilde{Q}_{n,r,e}^2) + (1 - p_n)^{-1}r_2^2(\tilde{Q}_{n,2r_1,2r_2-1,e} - \tilde{Q}_{n,r,e}^2),
\]

and define \( k_n := \max(K_n, 1/n) \). It follows from Theorem 2 and Slutsky’s theorem that \( k_n \) is a consistent estimator of the asymptotic variance \( \kappa \). Denote by \( H_n := \log(\max(\tilde{Q}_n, 1/n))/(1 - r) \), an estimator of \( h_r := \log(q_r)/(1 - r) \). Let \( L(n) \) be a slowly varying function. We obtain the following asymptotic result.
Theorem 3 Let \( p_X(x), p_Y(x) \in H^(\alpha)(C) \).

(i) Then the bias \( |\hat{q}_{r,\epsilon} - q_r| \leq C_1\epsilon^\alpha, C_1 > 0 \).

(ii) If \( 0 < \alpha \leq d/2 \) and \( \epsilon \sim cn^{-\alpha/(2\alpha+d(1-1/r))}, 0 < c < \infty \), then

\[
\hat{Q}_n - q_r = O_p(n^{-\alpha/(2\alpha+d(1-1/r))}) \quad \text{and} \quad H_n - h_r = O_p(n^{-\alpha/(2\alpha+d(1-1/r))}) \quad \text{as} \quad n \to \infty.
\]

(iii) If \( \alpha > d/2 \) and \( \epsilon \sim L(n)n^{-1/d} \) and \( ne^d \to \infty \), then

\[
\sqrt{n}(\hat{Q}_n - q_r) \overset{D}{\to} N(0, \kappa) \quad \text{and} \quad \sqrt{n}(\hat{Q}_n - q_r)/k_n^{1/2} \overset{D}{\to} N(0, 1);
\]

\[
\sqrt{n}(1 - r) \hat{Q}_n/k_n^{1/2}(H_n - h_r) \overset{D}{\to} N(0, 1) \quad \text{as} \quad n \to \infty.
\]

3 Applications and Numerical Experiments

3.1 Approximate Matching in Stochastic Databases

Let tables (in a relational database) \( T_1 \) and \( T_2 \) be matrices with \( m_1 \) and \( m_2 \) i.i.d. random tuples (or records), respectively. One of basic database operations, join, combines two tables into a third one by matching values for given columns (attributes). For example, the join condition can be the equality (equi-join) between a given pairs of attributes (e.g., names) from the tables. Joins are especially important for tying together pieces of disparate information scattered throughout a database (see, e.g., Kiefer et al. 2005, Copas and Hilton, 1990, and references therein). For the approximate join, we match \( \epsilon \)-close tuples, say, \( d(t_1(j), t_2(i)) \leq \epsilon, t_k(j) \in T_k, k = 1, 2, \) with a specified distance, see, e.g., Seleznjev and Thalheim (2008). A set of attributes \( A \) in a table \( T \) is called an \( \epsilon \)-key (test) if there are no \( \epsilon \)-close sub-tuples \( t_A(j), j = 1, \ldots, m \). Knowledge about the set of tests (\( \epsilon \)-keys) is very helpful for avoiding redundancy in identification and searching problems, characterizing the complexity of a database design for further optimization, see, e.g., Thalheim (2000). By joining a table with itself (self-join) we identify also \( \epsilon \)-keys and key-properties for a set of attributes for a random table (Seleznjev and Thalheim, 2003, Leonenko and Seleznjev, 2010).

The cost of join operations is usually proportional to the size of the intermediate results and so the joining order is a primary target of join-optimizers for multiple (large) tables, Thalheim (2000). The average case approach based on stochastic database modelling for optimization problems is proposed in Seleznjev and Thalheim (2008), where for random databases, the distribution of the \( \epsilon \)-join size \( N_\epsilon \) is studied. In particular, with some conditions it is shown that the average size

\[
EN_\epsilon = m_1m_2q_{1,1,\epsilon} = m_1m_2e^{db_1(d)(e^{-h_{1,1}} + o(1))} \quad \text{as} \quad \epsilon \to 0,
\]

that is the asymptotically optimal (in average) pairs of tables are amongst the tables with maximal value of the functional \( h_{1,1} \) (variability) and the corresponding estimators of \( h_{1,1} \) can be used for samples \( X_1, \ldots, X_{n_1} \) and \( Y_1, \ldots, Y_{n_2} \) from \( T_1 \) and \( T_2 \), respectively. For discrete distributions, similar results from Theorem 3 for \( \epsilon = 0 \) can be applied.

3.2 Image Matching using Quadratic-entropy Measures

Image retrieval and registration fall in the general area of pattern matching problems, where the best match to a reference or query image \( I_0 \) is to be found in a database of secondary images
The best match is expressed as a partial re-indexing of the database in decreasing order of similarity to the reference image using a similarity measure. In the context of image registration, the database corresponds to an infinite set of transformed versions of a secondary image, e.g., rotation and translation, which are compared to the reference image to register the secondary one to the reference.

Let $X$ be a $d$-dimensional random vector and let $p(x)$ and $q(x)$ denote two possible densities for $X$. In the sequel, $X$ is a feature vector constructed from the query image and a secondary image in an image database and $p(x)$ and $q(x)$ are densities, e.g., for the query image features and the secondary image features, respectively, say, image densities. When the features are discrete valued the $p(x)$ and $q(x)$ are probability mass functions.

The basis for entropy methods of image matching is a measure of similarity between image densities. A general entropy similarity measure is the Rényi $\alpha$-divergence, also called the Rényi $\alpha$-relative entropy, between $p(x)$ and $q(x)$

$$ D_\alpha(p, q) = \frac{1}{\alpha - 1} \log \int_{\mathbb{R}^d} q(x) (\frac{p(x)}{q(x)})^\alpha dx = \frac{1}{\alpha - 1} \log \int_{\mathbb{R}^d} p^\alpha(x)q^{1-\alpha}(x)dx, \quad \alpha \neq 1. $$

When the density $p(x)$ is supported on a compact domain and $q(x)$ is uniform over this domain, the Rényi $\alpha$-divergence reduces to the Rényi $\alpha$-entropy

$$ h_\alpha(p) = \frac{1}{1 - \alpha} \log \int_{\mathbb{R}^d} p^\alpha(x)dx. $$

Another important example of statistical distance between distributions is given by the following nonsymmetric Bregman distance (see, e.g., Pardo, 2006)

$$ B_s(p, q) = \int_{\mathbb{R}^d} [q(x)^s + \frac{1}{s-1}p(x)^s - \frac{s}{s-1}p(x)q(x)^{s-1}] dx, \quad s \neq 1, $$

or its symmetrized version

$$ K_s(p, q) = \frac{1}{s} [B_s(p, q) + B_s(q, p)] = \frac{1}{s - 1} \int_{\mathbb{R}^d} [p(x) - q(x)][p(x)^{s-1} - q(x)^{s-1}]dx. $$

For $s = 2$, we get the second order distance

$$ B_2(p, q) = K_2(p, q) = \int_{\mathbb{R}^d} [p(x) - q(x)]^2 dx. $$

Now, for an integer $s$, applying Theorem 1 and 3 one can obtain an asymptotically normal estimator of the Rényi $s$-entropy and a consistent estimator of the Bregman distance.

### 3.3 Entropy Maximizing Distributions

For a positive definite and symmetric matrix $\Sigma$, $s \neq 1$, define the constants

$$ m = d + 2/(s - 1), \quad C_s = (m + 2)\Sigma, $$

and

$$ A_s = \frac{1}{|\pi C_s|^{1/2}} \frac{\Gamma(m/2 + 1)}{\Gamma((m - d)/2 + 1)}. $$
Among all densities with mean $\mu$ and covariance matrix $\Sigma$, the Rényi entropy $h_s$, $s = 2, \ldots$, is uniquely maximized by the density (Costa et al. 2003)

$$p_s^*(x) = \begin{cases} A_s(1 - (x - \mu)^T C_s^{-1}(x - \mu))^{1/(s-1)}, & x \in \Omega_s \\ 0, & x \notin \Omega_s, \end{cases}$$

with support

$$\Omega_s = \{ x \in \mathbb{R}^d : (x - \mu)^T C_s^{-1}(x - \mu) \leq 1 \}.$$

The distribution given by $p_s^*(x)$ belongs to the class of Student-$r$ distributions. Let $\mathcal{K}$ be a class of $d$-dimensional density functions $p(x), x \in \mathbb{R}^d$, with positive definite covariance matrix. By the procedure described in Leonenko and Seleznjev (2010), the proposed estimator of $h_s$ can be used for distribution identification problems, i.e., to test the null hypothesis $H_0 : X_1, \ldots, X_n$ is a sample from a Student-$r$ distribution of type (1) against the alternative $H_1 : X_1, \ldots, X_n$ is a sample from any other member of $\mathcal{K}$.

### 3.4 Numerical Experiments

**Example 1.** Figure 1 shows the accuracy of the estimator for the cubic Rényi entropy $h_{3,0}$ of discrete distributions in Theorem 1 for a sample from a $d$-dimensional Bernoulli distribution and $n$ observations, $d = 3$, $n = 300$, with Bernoulli $Be(p)$-i.i.d. components, $p = 0.8$. Here the coincidence probability $q_{3,0} = (p^3 + (1 - p)^3)^3$ and the Rényi entropy $h_{3,0} = -\log(q_{3,0})/2$. The histogram for the normalized residuals $r_{ni} := 2\sqrt{n}Q_n(H_n - h)_{r_i}/k_n^{1/2}, i = 1, \ldots, N_{sim}$ are compared to the standard normal density, $N_{sim} = 500$. The corresponding qq-plot and p-values for the Kolmogorov-Smirnov (0.4948) and Shapiro-Wilk (0.7292) tests also support normality hypothesis for the obtained residuals.

![Histogram of residuals](image1.png)

![Normal Q-Q Plot](image2.png)

Figure 1: Bernoulli $d$-dimensional distribution; $d = 3$, $Be(p)$-i.i.d. components, $p = 0.8$, sample size $n = 200$. Standard normal approximation for the empirical distribution (histogram) for the normalized residuals, $N_{sim} = 500$. 
Example 2. Figure 2 illustrates the performance of the approximation for the differentiable variability \( v = h_{1,1} \) in Theorem 2 for two one-dimensional samples from normal distributions \( N(0, 3/2) \) and \( N(2, 1/2) \), with the sample sizes \( n_1 = 100, n_2 = 200 \), respectively. Here the variability \( v = \log(2\sqrt{\pi e}) \). The normalized residuals are compared to the standard normal density, \( N_{sim} = 300 \). The qq-plot and p-values for the Kolmogorov-Smirnov (0.9916) and Shapiro-Wilk (0.5183) tests also support the normal approximation.

Figure 2: Two Gaussian distributions; \( N(0, 3/2), N(2, 1/2), n_1 = 100, n_2 = 200, \epsilon = 1/10 \). Standard normal approximation for the empirical distribution (histogram) for the normalized residuals, \( N_{sim} = 300 \).

Example 3. Figure 3 shows the accuracy of the normal approximation for the cubic Rényi entropy \( h_{3,0} \) in Theorem 3 for a sample from a bivariate Gaussian distribution with \( N(0,1) \)-i.i.d. components, and \( n = 300 \) observations. Here the Rényi entropy \( h_{3,0} = \log(\sqrt{12\pi}) \). The histogram, qq-plot, and p-values for the Kolmogorov-Smirnov (0.2107) and Shapiro-Wilk (0.2868) tests allow to accept the hypothesis of standard normality for the residuals, \( N_{sim} = 300 \).

Example 4. Figure 4 demonstrates the behaviour of the estimator for the quadratic Bregman distance \( B_2(p, q) \) for two exponential distributions \( p(x) = \beta_1 e^{-\beta_1 x}, x > 0 \), and \( q(x) = \beta_2 e^{-\beta_2 x}, x > 0 \), with rate parameters \( \beta_1 = 1, \beta_2 = 3 \), respectively, and equal sample sizes. Here the Bregman distance \( B_2(p, q) = 1/2 \). The empirical mean squared error (MSE) based on 10000 independent simulations are calculated for different values of \( n \).

4 Proofs

Lemma 1 Assume that \( p_X(x) \) and \( p_Y(x) \) are bounded and continuous or with a finite number of discontinuity points. Let \( a, b \geq 0 \). Then

\[
b_\epsilon(d)^{-(a+b)} E(p_{X,\epsilon}(X)^a p_{Y,\epsilon}(X)^b) \to \int_{R^d} p_X(x)^{a+1} p_Y(x)^b dx \text{ as } \epsilon \to 0.
\]
Figure 3: Bivariate normal distribution with \( N(0, 1) \)-i.i.d. components; sample size \( n = 300, \epsilon = 1/2 \). Standard normal approximation for the empirical distribution (histogram) for the normalized residuals, \( N_{\text{sim}} = 300 \).

Proof: We have

\[ b_\epsilon(d)^{-a-b} E(p_{X_\epsilon}(X)^a p_{Y_\epsilon}(X)^b) = E(g_\epsilon(X)), \]

where \( g_\epsilon(x) := (p_{X_\epsilon}(x)/b_\epsilon(d))^a (p_{Y_\epsilon}(x)/b_\epsilon(d))^b \). It follows by definition that \( g_\epsilon(x) \to p_X(x)^a p_Y(x)^b \) as \( \epsilon \to 0 \), for all continuity points of \( p_X(x) \) and \( p_Y(x) \), and that the random variable \( g_\epsilon(X) \) is bounded. Hence, the bounded convergence theorem implies

\[ E(g_\epsilon(X)) \to E(p_X(X)^a p_Y(X)^b) = q_{a+1,b} \text{ as } \epsilon \to 0. \]

\[ \Box \]

Proof of Theorem: (i) Note that for \( k = 1, \ldots, r_1 \),

\[ n_{k,\epsilon}(d-1) = (n_{1,\epsilon}(1-1/k))^{k} \geq (n_{1,\epsilon}(1-1/r))^{k} \geq n_{1,\epsilon}(1-1/r). \]  

(2)

We use the conventional results from the theory of \( U \)-statistics (see, e.g., Lee, 1990, Koroljuk and Borovskich, 1994). For \( l = 0, \ldots, r_1 \), and \( m = 0, \ldots, r_2 \), define

\[ \psi_{l,m,n}(x_1, \ldots, x_l; y_1, \ldots, y_m) := E(\psi_n(x_1, \ldots, x_l, X_{l+1}, \ldots, X_{r_1}; y_1, \ldots, y_m, Y_{m+1}, \ldots, Y_{r_2})) \]

\[ = \frac{1}{r_1} \sum_{i=1}^{r_1} E(\psi_n^{(i)}(x_1, \ldots, x_l, X_{l+1}, \ldots, X_{r_1}; y_1, \ldots, y_m, Y_{m+1}, \ldots, Y_{r_2})), \]

(3)

and

\[ \sigma^2_{l,m,\epsilon} := \text{Var}(\psi_{l,m,n}(X_1, \ldots, X_l; Y_1, \ldots, Y_m)). \]

Let \( S_1, S_2 \in S_{n_1, r_1} \) and \( T_1, T_2 \in S_{n_2, r_2} \) have \( l \) and \( m \) elements in common, respectively. By properties of \( U \)-statistics, we have

\[ v^2_n = \text{Var}(\tilde{Q}_n) = b_\epsilon(d)^{-2(\epsilon-1)} \sum_{l=0}^{r_1} \sum_{m=0}^{r_2} \binom{r_1}{l} \binom{r_2}{m} \binom{m_{1-l}}{r_1} \binom{m_{2-m}}{r_2} \sigma^2_{l,m,\epsilon}, \]

(4)
Figure 4: Bregman distance for $\text{Exp}(\beta_1)$ and $\text{Exp}(\beta_2)$, $\beta_1 = 1$, $\beta_2 = 3$. The empirical MSE obtained for the $U$-statistic estimator with $n\epsilon = a$, for different values of $a$.

and

$$\sigma^2_{l,m,\epsilon} = \text{Cov}(\psi_n(S_1; T_1), \psi_n(S_2; T_2)).$$  \hspace{1cm} (5)

From (5) we get that $0 \leq \sigma^2_{l,m,\epsilon} \leq E(\psi_n(S_1; T_1)\psi_n(S_2; T_2))$, which is a finite linear combination of $P(A_i \cap A_j)$, $i \in S_1, j \in S_2$, where

$$A_i := \{d(X_i, X_k) \leq \epsilon, d(X_i, Y_s) \leq \epsilon, \forall k \in S_1, \forall s \in T_1\}.$$

When $l \neq 0$ or $m \neq 0$, the triangle inequality implies that

$$A_i \cap A_j \subseteq F_i := \{d(X_i, X_k) \leq 3\epsilon, d(X_i, Y_s) \leq 3\epsilon, \forall k \in S_1 \cup S_2, \forall s \in T_1 \cup T_2\},$$

and since $|S_1 \cup S_2| = 2r_1 - l$ and $|T_1 \cup T_2| = 2r_2 - m$, it follows by conditioning and from Lemma 1 that

$$P(A_i \cap A_j) \leq P(F_i) = E(p_{X,3\epsilon}(X_i)^{2r_1-l-1}p_{Y,3\epsilon}(X_i)^{2r_2-m}) \sim 3^{d(2r-l-m-1)}b_\epsilon(d)^{2r-l-m-1}q_{2r_1-l,2r_2-m} \text{ as } n \rightarrow \infty.$$  \hspace{1cm} (7)

We conclude that

$$\sigma^2_{l,m,\epsilon} = O(b_\epsilon(d)^{2r-l-m-1}) \text{ as } n \rightarrow \infty. \hspace{1cm} (6)$$

Now, for $l = 0, \ldots, r_1$ and $m = 0, \ldots, r_2$, we obtain

$$b_\epsilon(d)^{-2(r-1)} \binom{r_1}{m} \binom{r_2}{m} \binom{n_1-r_1}{r_1-l} \binom{n_2-r_2}{r_2-m} \sigma^2_{l,m,\epsilon} \sim C_{l,m} \frac{b_\epsilon(d)^{-(2r-l-m-1)}\sigma^2_{l,m,\epsilon}}{n^{l+m-d(l+m-1)}} \text{ as } n \rightarrow \infty, \hspace{1cm} (7)$$
for some constant $C_{l,m} > 0$. Hence, from (2), (4), (5), and (7) we get that $\tau_n^2 = O((ne^{d(1-1/r)})^{-1})$ as $n \to \infty$. Moreover, it follows from Lemma 1 that $E\hat{Q}_n \to q_r$ as $n \to \infty$, so when $ne^{d(1-1/r)} \to \infty$, then

$$E(\hat{Q}_n - q_r)^2 = \tau_n^2 + (E(\hat{Q}_n - q_r))^2 \to 0,$$

and the assertion follows.

(ii) Let

$$h_n^{(1,0)}(x) := \psi_{1,0,n}(x)/b_e(d)^{r-1} - \tilde{q}_{r,\epsilon}, \quad h_n^{(0,1)}(x) := \psi_{0,1,n}(x)/b_e(d)^{r-1} - \tilde{q}_{r,\epsilon}. \quad (8)$$

The H-decomposition of $\hat{Q}_n$ is given by

$$\hat{Q}_n = \tilde{q}_{r,\epsilon} + r_1 H_n^{(1,0)} + r_2 H_n^{(0,1)} + R_n, \quad (9)$$

where

$$H_n^{(1,0)} := \frac{1}{n_1} \sum_{i=1}^{n_1} h_n^{(1,0)}(X_i), \quad H_n^{(0,1)} := \frac{1}{n_2} \sum_{i=1}^{n_2} h_n^{(0,1)}(Y_i).$$

The terms in (9) are uncorrelated, and since $\text{Var}(h_n^{(1,0)}(X_1)) = b_e(d)^{-2(r-1)}\sigma_{1,0,\epsilon}^2$ and $\text{Var}(h_n^{(0,1)}(Y_1)) = b_e(d)^{-2(r-1)}\sigma_{0,1,\epsilon}^2$, we obtain (10) that

$$\text{Var}(R_n) = \text{Var}(\hat{Q}_n) - \text{Var}(r_1 H_n^{(1,0)}) - \text{Var}(r_2 H_n^{(0,1)})$$

$$= \text{Var}(\hat{Q}_n) - b_e(d)^{-2(r-1)}r_1^2n_1^{-1}\sigma_{1,0,\epsilon}^2 - b_e(d)^{-2(r-1)}r_2^2n_2^{-1}\sigma_{0,1,\epsilon}^2$$

$$= K_{1,n}b_e(d)^{-2(r-1)}n^{-1}\sigma_{1,0,\epsilon}^2 + K_{2,n}b_e(d)^{-2(r-1)}n^{-1}\sigma_{0,1,\epsilon}^2$$

$$+ b_e(d)^{-2(r-1)} \sum_{E} \left( \frac{r_1}{n_1} \right) \left( \frac{r_2}{n_2} \right) \left( \frac{r_1 - 1}{n_1 - 1} \right) \left( \frac{r_2 - 1}{n_2 - 1} \right) \sigma_{l,m,e}^2.$$  

(10)

where $E := \{(l, m) : 0 \leq l \leq r_1, 0 \leq m \leq r_2, l + m \geq 2\}$, and

$$K_{1,n} := \frac{r_1^2}{p_n} \left( \frac{r_1 - 1}{n_1 - 1} \right) \left( \frac{r_2 - 1}{n_2 - 1} \right) - 1,$$

$$K_{2,n} := \frac{r_2^2}{1 - p_n} \left( \frac{r_1 - 1}{n_1 - 1} \right) \left( \frac{r_2 - 1}{n_2 - 1} \right) - 1.$$

Note that $K_{1,n}, K_{2,n} = O(n^{-1})$ as $n \to \infty$ so if $ne^{d} \to a, 0 < a \leq \infty$, then (7), (8), and (10) imply that $\text{Var}(R_n) = O((n^2e^d)^{-1})$ as $n \to \infty$. In particular, for $a = \infty$,

$$\text{Var}(R_n) = o(n^{-1}) \Rightarrow n^{1/2}R_n \to 0 \quad \text{as} \quad n \to \infty.$$  

(11)

By symmetry, we have from (3)

$$\psi_{1,0,n}(x) = \frac{1}{r_1} \left( p_{X,\epsilon}(x)^{r_1 - 1}p_{Y,\epsilon}(x)^{r_2} + (r_1 - 1)E(\psi_n^{(2)}(x, X_2, \ldots, X_{r_1}; Y_1, \ldots, Y_{r_2})) \right). \quad (12)$$

Let $x$ be a continuity point of $p_X(x)$ and $p_Y(x)$. Then, changing variables $y = x + \epsilon u$ and the bounded convergence theorem give

$$E(\psi_n^{(2)}(x, X_2, \ldots, X_{r_1}; Y_1, \ldots, Y_{r_2}) = E(E(\psi_n^{(2)}(x, X_2, \ldots, X_{r_1}; Y_1, \ldots, Y_{r_2})|X_2))$$

$$= \int_{R^d} I(d(x, y) \leq \epsilon)p_{X,\epsilon}(y)^{r_1 - 2}p_{Y,\epsilon}(y)^{r_2}p_X(x)dy$$

$$= \epsilon^d \int_{R^d} I(d(0, u) \leq \epsilon)p_{X,\epsilon}(x + \epsilon u)^{r_1 - 2}p_{Y,\epsilon}(x + \epsilon u)^{r_2}p_X(x + \epsilon u)du$$

$$\sim b_e(d)^{-r_1}p_X(x)^{-r_1}p_Y(x)^{r_2} \quad \text{as} \quad n \to \infty.$$  

(13)
From (12) we get that
\[ \psi_{1,0,n}(x) \sim b_ε(d)r^{-1}p_X(x)^{r_1-1}p_Y(x)^{r_1} \text{ as } n \to \infty, \]
and hence
\[ \lim_{n \to \infty} h_n^{(1,0)}(x) = p_X(x)^{r_1-1}p_Y(x)^{r_2} - q_r, \tag{14} \]
and similarly,
\[ \lim_{n \to \infty} h_n^{(0,1)}(x) = p_X(x)^{r_1}p_Y(x)^{r_2-1} - q_r. \tag{15} \]

Let $\max(p_X(x), p_Y(x)) \leq C, x \in R^d$. Then $\max(p_{X,ε}(x), p_{Y,ε}(x)) \leq b_ε(d)C, x \in R^d$. It follows from (12) and (13) that $\psi_{1,0,n}(x) \leq b_ε(d)r^{-1}C^{r-1}, x \in R^d$, and hence $h_n^{(1,0)}(x) \leq 2C^{r-1}, x \in R^d$.

Similarly, we have that $h_n^{(0,1)}(x) \leq 2C^{r-1}, x \in R^d$. Therefore, $h_n^{(1,0)}(X_1)$ and $h_n^{(0,1)}(Y_1)$ are bounded random variables. Hence, from (14), (15), and the bounded convergence theorem we obtain
\[
\text{Var}(h_n^{(1,0)}(X_1)) \to ζ_{1,0}, \quad \text{Var}(h_n^{(0,1)}(Y_1)) \to ζ_{0,1} \text{ as } n \to \infty.
\]

Let $Z_{n,i} := n_i^{-1/2}h_n^{(1,0)}(X_i), i = 1, \ldots, n_1$, and observe that, for $δ > 0$,
\[
\sum_{i=1}^{n_1} E Z_{n,i}^2 = \text{Var}(h_n^{(1,0)}(X_1)) \to ζ_{1,0} > 0 \text{ as } n \to \infty,
\]

\[
\lim_{n \to \infty} \sum_{i=1}^{n_1} E(|Z_{n,i}|^2I(|Z_{n,i}| > δ)) = \lim_{n \to \infty} E(|h_n^{(1,0)}(X_1)|^2I(|h_n^{(1,0)}(X_1)| > δn_1^{1/2})) \leq \lim_{n \to \infty} 4C^{2(r-1)}E(I(|h_n^{(1,0)}(X_1)| > δn_1^{1/2})) = 0,
\]

where the last equality follows from the boundedness of $h_n^{(1,0)}(X_1)$. The Lindeberg-Feller Theorem (see, e.g., Theorem 4.6, Durrett, 1991) gives that
\[ Z_{n,1} + \ldots + Z_{n,n_1} = n_1^{1/2}H_n^{(1,0)} \overset{D}{\to} N(0, ζ_{1,0}) \text{ as } n \to \infty, \]
and similarly $n_2^{1/2}H_n^{(0,1)} \overset{D}{\to} N(0, ζ_{0,1}) \text{ as } n \to \infty$. Hence, by independence we get that
\[ n^{1/2}(r_1H_n^{(1,0)} + r_2H_n^{(0,1)}) \overset{D}{\to} N(0, κ) \text{ as } n \to \infty, \]
so from (11) and Slutsky’s theorem,
\[ n^{1/2}(\tilde{q}_n - q_r,ε) = n^{1/2}(r_1H_n^{(1,0)} + r_2H_n^{(0,1)}) + n^{1/2}R_n \overset{D}{\to} N(0, κ) \text{ as } n \to \infty. \]

This completes the proof. \( \square \)

Proof of Theorem 4: The proof is similar to that of the corresponding result in Leonenko and Seleznjev (2010) so we give the main steps only. First we evaluate the bias term $B_n := \tilde{q}_r,ε - q_r$. 

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Let $V := (V_1, \ldots, V_d)'$ be an auxiliary random vector uniformly distributed in the unit ball $B_1(0)$, say, $V \in U(B_1(0))$. Then by definition, we have

$$B_n = \int_{R^d} p_{X,\epsilon}(x)^{r_1-1}p_Y(x)^{r_2}p_X(x)dx - \int_{R^d} p_X(x)^{r_1}p_Y(x)^{r_2}dx = E(D_n(X)),$$

where

$$D_n(x) := p_{X,\epsilon}(x)^{r_1-1}p_Y(x)^{r_2} - p_X(x)^{r_1-1}p_Y(x)^{r_2} = p_{X,\epsilon}(x)^{r_1-1}(p_Y(x)^{r_2} - p_Y(x)^{r_2}) + p_Y(x)^{r_2}(p_{X,\epsilon}(x)^{r_1-1} - p_X(x)^{r_1-1}).$$

It follows by definition that

$$D_n(x) = P_1(x)(p_{X,\epsilon}(x) - p_Y(x)) + P_2(x)(p_{X,\epsilon}(x) - p_X(x)) = E(P_1(x)(p_Y(x - \epsilon V) - p_Y(x)) + P_2(x)(p_X(x - \epsilon V) - p_X(x)))$$

where $P_1(x)$ and $P_2(x)$ are polynomials in $p_X(x), p_Y(x), E(p_X(x - \epsilon V)), \text{ and } E(p_Y(x - \epsilon V))$. Now the boundedness of $p_X(x)$ and $p_Y(x)$ and the Hölder condition for the continuous differentiable cases imply

$$|D_n(x)| \leq CC_1 \epsilon^\alpha, C_1 > 0,$$

and the assertion (i) follows.

For $\epsilon \sim cn^{-1/(2\alpha + d(1-1/r))}, 0 < c < \infty, \alpha < d/2$, by (i) and Theorem 1, we have

$$B_n^2 + v_n^2 = O(n^{-2\alpha/(2\alpha + d(1-1/r))}).$$

Now for some $C > 0$ and any $A > 0$ and large enough $n_1, n_2$, we obtain

$$P \left( \left| \hat{Q}_n - q_r \right| > An^\alpha/(2\alpha + d(1-1/r)) \right) \leq n^{-2\alpha/(2\alpha + d(1-1/r))} \frac{B_n^2 + v_n^2}{A^2} \leq \frac{C}{A^2},$$

and the assertion (ii) follows. Similarly for $\alpha = d/2$.

Finally, for $\alpha > d/2$ and $\epsilon \sim L(n)n^{-1/d}$ and $n\epsilon^d \to \infty$, the assertion (iii) follows from Theorem 2 and the Slutsky theorem. This completes the proof. \qed

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