# **Ensembles of Nonparametric Entropy Estimators**

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### 1 Introduction

- 2 Information entropy is the average amount of information produced by a random variable. Shannon (1949)
- defines the differential entropy H of a random variable X and probability mass function p(x) as

$$H(X) = -\int p(x)\log p(x)dx$$

- Since the true probability is not known, it is not possible to calculate H(X) directly.
- 6 Entropy estimation has many important applications. For example, it can be used to estimate the mutual
- 7 information of two random variables and provide insights about their relationship. Furthermore, information
- 8 entropy has other applications in encoding data, data compression, clustering, and a criterion for feature-
- 9 splitting in decision trees.
- 10 Entropy estimation is difficult because it requires estimating the non-smooth function  $f(x) = -x \log(x)$ , that
- is not differentiable at x=0. One approach is to use the naive plugin estimator from the empirical distribution
- 12 and get

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$$\hat{H}(X) = -\sum_{i=1}^{n} \hat{p}(x_i) \log \hat{p}(x_i)$$

- where  $\hat{p}(x_i) = \frac{h_i}{n}$  is the MLE of each probability  $p(x_i)$  and  $h_i = \sum_{k=1}^n \mathbb{I}(X_k = i)$  is the histogram over the
- 15 outcomes.
- 16 However, Basharin (1959) and Harris (1975) have shown that the naive plugin estimator always underestimates
- the true entropy. Another result from Paninski (2003) proves that there exists no unbiased estimator for entropy.
- Furthermore, many of the existing estimators suffer from the curse of dimensionality and converge slowly at
- the rate of  $O(T^{-\gamma/d})$  where T is the number of samples and  $\gamma$  is a positive rate parameter.
- 20 In this paper, we will summarize the results of some well-known entropy estimators as well as a weighted
- ensemble method that, under the right conditions, can remove the dependency on the dimension and ensure
- 22 a convergence rate of  $O(T^{-1})$ . At the end, we will also discuss the results concerning the minimax rate of
- 23 entropy estimators.

# 24 **2** Entropy Estimation Overview

# 25 2.1 Plug-in Estimators

- Beirlant et al. [1] gives an overview of several popular methods for the nonparametric estimation of entropy.
- 27 Besides the MLE plug-in estimator, there are other plug-in estimators that utilize techniques such as kernel
- density estimation, splitting data, or cross-validation.
- Consider  $X_1,...X_n$  and an estimator of the form  $H_n = -\frac{1}{n}\sum_{i=1}^n \log f_n(X_i)$  where  $f_n$  is a **kernel density**
- estimator. Joe (1989) shows that the MSE converges at the rate  $O(n^{-1}) + O(n^{-2}h^{8-d}) + O(n^{-2}h^{-d}) + O(n^{-2}h^{-d})$
- $O(n^{-1}h^{8-d})+O(n^{-2}h^{4-2d})+O(h^8)$  where n is the sample size, h is the binwidth, and d is the dimension.
- The analysis shows that the sample size that is needed for good estimators increases rapidly with the dimension
- of the multivariate density.

- Another plug-in estimator is the **splitting-data estimator**. Start by decomposing the sample into two sets:
- $X_1,...,X_i$  and  $X_{i+1*},...,X_{n*}$ . Using the first set of data, construct a density estimate  $f_i$  and then, using  $f_i$
- and the second set, construct  $H_n = -\frac{1}{n (i + 1)} \sum_{j=i+1}^n \mathbb{I}_{X_{j*}} \log f_j(X_j*)$ . For  $f_j$  being the histogram density
- estimate, kernel density estimate, and any  $L_1$ -consistent density estimator, Gyorfi and van der Meulen (1987, 37
- 1989, 1990) show that the estimator  $H_n$  converges almost surely to H(f) under some mild tail and smoothness 38
- condition.
- The final plug-in estimator is based on **cross-validation**. Let  $f_{n,i}$  denotes the kernel density estimator based
- on  $X_1, ..., X_n$  leaving  $X_i$  out, then the corresponding density estimator is  $H_n = -\frac{1}{n} \sum_{i=1}^n \mathbb{I}_{X_i} \log f_{n,i}(X_i)$ .

# **Estimators using Nearest Neighbors**

- Another interesting technique to estimate entropy is by using the nearest neighbor distances. Let  $\rho_{n,i}$  be the nearest neighbor distance of  $X_i$  and the other  $X_j: \rho_{n,i} = \min_{j \neq i, j \leq n} ||X_i X_j||$ . The nearest neighbor
- estimate is  $H_n = \frac{1}{n} \sum_{i=1}^n \ln(n\rho_{n,i}) + \ln(2) + C_E$  where the Euler constant  $C_E = -\int_0^\infty e^{-t} \ln(t) dt$ .

#### Results 3

- The estimators mentioned above can converge at a very slow rate as the dimension grows large. Sricharan
- et al. [2] propose a weighted density functionals estimator that takes the weighted affine combination of an
- ensemble of slow functional estimators to estimate entropy. The ensemble, under the right conditions, can 49
- converge at a rate that is independent of the dimension. 50
- Result 1: MSE rate of the weighted ensemble of estimators 51
- Let T be the total sample size,  $\gamma$  be a positive rate parameter, and d be the dimension. Sricharan et al. [2] 52
- show that an ensemble of slow estimators with the MSE decay rate of order  $O(T^{-\gamma/d})$  can converge at a much 53
- faster dimension-invariant rate of O(1/T). 54
- Result 2: Entropy estimation using a weighted ensemble of truncated uniform kernel density estimators
- They also apply this weighted estimator, with an ensemble of truncated uniform kernel density estimators, to
- the problem of Shannon entropy estimation and show that it performs better than many well-known plugin 57
- estimators, especially in higher dimensions. Specifically, the weighted ensemble estimator can estimate entropy 58
- at  $O(T^{-1})$  convergence rate. 59
- Result 3: Entropy estimation using a weighted ensemble of k-nearest neighbors estimators 60
- Gao et al [3] show that k-NN based multivariate entropy estimators [4] achieve parametric MSE rate when the 61
- dimension of each of the random variables is less than 3. However, for larger dimensions, Singh and Poczos 62
- [5] derive the convergence rates for fixed k-NN entropy estimators. It is shown that the bound on the bias of the
- estimator is given by  $O(\frac{k}{T}^{\beta/D})$ , where k is the numbers of neighbors evaluated,  $\beta$  is a measure of the Hölder smoothness of the sampling density, and  $D \leq d$  is the intrinsic dimension of the support of the distribution. 64
- 65
- Since k and  $\beta$  can be set to a constant values and D < d, the bias can be further bounded by  $O(T^{-d})$ . The
- variance of the estimator is also shown to be bounded by  $O(T^{-1})$ , so we now have the desirable properties to
- calculate a weighted ensemble of these k-NN based entropy estimators with parametric MSE rate of  $O(T^{-1})$ . 68
- Result 4: Minimax rate of entropy estimator 69
- Finally, we look at the minimax rate of estimating integral functions in general. Birge and Massart [6] extend
- a minimax rate result to estimating functions of the general form  $\int \phi(f(x), f'(x), ..., f^{(k)}(x), x) dx$  where f 71
- has some density smoothness s. Given the critical index of smoothness  $s_c = 2k + d/4$ , if  $s > s_c$  then an estimator can be constructed to obtain a convergence rate of  $O(\frac{1}{\sqrt{n}})$ . Otherwise, it is not possible to estimate 72
- at a better rate than  $O(\frac{1}{n^{\gamma}})$  where  $\gamma = 4s/(4s+d)$  for d > 1.

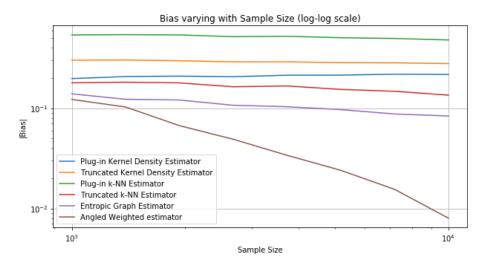


Figure 1: MSE rates for entropy estimators as a function of sample size

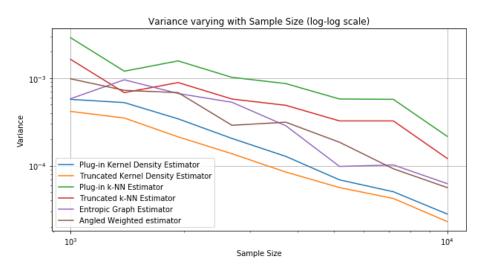


Figure 2: Magnitude of bias for entropy estimators as a function of sample size

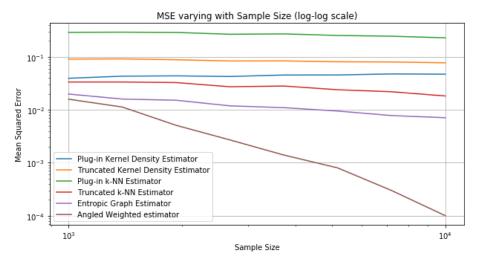


Figure 3: Variance for entropy estimators as a function of sample size

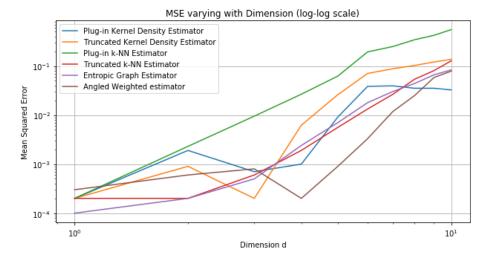


Figure 4: MSE rates for entropy estimators as a function of sample dimension

# 4 Experiments

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Sricharan et al. [2] observe that the weighted ensemble of truncated kernel density estimators achieve meansquared error rates better than other popular entropy estimators, including the kernel density estimator [7], truncated kernel density estimator, k-NN based Kozachenko-Leonenko estimator [8], truncated KL estimator, and the entropic graph estimator [9].

We used the aforementioned estimators to approximate the Shannon entropy for testing the probability distribution of a random sample and show the MSE rates for each estimator as a function of sample size T in Figure 3, for fixed dimension d=6. We can see that the weighted ensemble estimator achieves better error rates than those of other estimators. The ensemble converges faster for the bias, whereas for the variance, it converges at a rate similar to those of the other estimators. The experimental results follow our derived results for the bias and variance bounds of the truncated kernel density estimator, weighted estimator, and k-NN based KL estimator—we get similar  $O(T^{-1})$  variance bounds for the three estimators, but the weighted estimator achieves a lower bias bound which is independent on the dimension of the data.

We also tried to reproduce the MSE rate results from [2] by varying the sample data dimension d with fixed sample size of 3000 in Figure 4, but were not able to achieve the noticeably superior performances reported in the paper. Specifically, the MSE rates for the weighted entropy estimator deteriorates when d > 8. We still observed the expected MSE rate behavior for  $d \le 8$  in that the weighted estimator performs worse than other entropy estimators in lower dimensions, but does better in higher dimensions—this is because the MSE rates for the other estimators depend on d, and thus suffer from curse of dimensionality as d increases.

# 5 Outline of Proofs

### 5.1 MSE rate of the weighted ensemble of estimators

We define our ensemble estimator as  $\hat{\mathbf{E}}_w = \sum_{l \in \bar{l}} w(l) \hat{\mathbf{E}}_l$ , where  $\bar{l}$  denotes the set of parameters and  $\hat{\mathbf{E}}_l$  are the L parameterized, unbiased estimators. We also add the weights constraint that  $\sum_{l \in \bar{l}} w(l) = 1$ , which guarantees that the weighted estimator will be asymptotically unbiased. For each  $\hat{\mathbf{E}}_l$ , we assume that bias and variance is given by:

$$\mathbb{B}(\hat{\mathbf{E}}_l) = \sum_{i \in [I]} c_i \psi_i(l) T^{-i/2d} + O\left(\frac{1}{\sqrt{T}}\right)$$
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$$\mathbb{V}(\hat{\mathbf{E}}_t) = c_v\left(\frac{1}{T}\right) + o\left(\frac{1}{T}\right)$$

where  $c_i$  and  $c_v$  are constants, I is a finite index set with cardinality I < L, and  $\psi_i(l)$  are basis functions which only depend on l.

104 *Proof*: With above bias and variance conditions, a weight vector  $w_0$  can be found by solving a convex optimization problem such that  $\mathbb{E}[(\hat{\mathbf{E}}_{w_o} - E)^2] = O(1/T)$ . The optimization problem is defined as:

$$\begin{array}{rcl} \min\limits_{w} & ||w||_2 \\ \text{subject to } \sum\limits_{l\in \bar{l}} w(l) & = & 1, \\ \\ \gamma_w(i) & = & \sum\limits_{l\in \bar{l}} w_l \psi_i(l) = 0, i\in [I], \end{array}$$

From this setting, the bias and variance of the weighted estimator can be calculated as:

$$\mathbb{B}(\hat{\mathbf{E}}_w) = \sum_{i \in I} c_i \gamma_w(i) T^{-i/2d} + O\left(\frac{||w||_1}{\sqrt{T}}\right)$$
$$= \sum_{i \in I} c_i \gamma_w(i) T^{-i/2d} + O\left(\frac{\sqrt{L}||w||_2}{\sqrt{T}}\right)$$

Denote the covariance matrix  $\{\hat{\mathbf{E}}_l; l \in \bar{l}\}$  by  $\Sigma_L$ . Let  $\bar{\Sigma}_L = \Sigma_L T$ ,

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$$\mathbb{V}(\hat{\mathbf{E}}_w) = \mathbb{V}\left(\sum_{l \in \bar{l}} w_l \hat{\mathbf{E}}_l\right) = w^T \Sigma_L w = \frac{w^T \bar{\Sigma}_L w}{T} \le \frac{L||w||_2^2}{T}$$

We can also rewrite the earlier convex optimization constraints in matrix form as  $\min_{w} ||w||_2^2$  subject to  $A_0w = b$ , where b is vector of zeros with a leading one and  $A_0$  is the basis projection matrix—where first row is a vector of ones and the  $i^{th}$  row  $(A_0)_i = [\psi_i(l_1), ..., \psi_i(l_L)]$ . Also, let  $A_1$  be the  $A_0$  matrix without the first row of ones, then solving for the minimum square norm  $\eta_L(d) := ||w_0||_2^2$  is given by  $\eta_L(d) = \frac{\det(A_1A_1')}{\det(A_0A_0')}$ 

where  $\eta_L(d)$  is independent of T given fixed number of estimators L and fixed dimension d, i.e.  $\eta_L(d) = \Theta(1)$ .

The bias and variance of the weighted estimator is therefore:

$$\mathbb{B}[\hat{\mathbf{E}}_{w_0}] = O\left(\sqrt{L\eta_L(d)/T}\right) = O\left(1/\sqrt{T}\right)$$

$$\mathbb{V}[\hat{\mathbf{E}}_{w_0}] = O(L\eta_L(d)/T) = O(1/T)$$

Thus, the overall MSE rate converges in dimension invariant rate of O(1/T).

# 5.2 Entropy estimation using a weighted ensemble of truncated uniform kernel density estimators

We can now estimate any general d-dimensional, non-linear density functionals of the form

$$G(f) = \int g(f(x), x) f(x) dx.$$

Let T = N + M and represent the i.i.d observations from f as  $\{X_1, ..., X_N, X_{N+1}, ..., X_{N+M}\}$ . We have shown an ensemble estimator that will converge much faster than their slower estimator components, if they match the bias and variance conditions. We present one such plugin estimator called the truncated uniform kernel density estimator:

$$\hat{f}_k(X) = \frac{\sum_{i=1}^{M} \mathbb{I}_{\{X_i \in S_k(X)\}}}{MV_k(X)}$$

where  $k \leq M$  is a real number,  $S_k(X)$  is the truncated kernel region for each X in finite support  $[a,b]^d$ , and  $V_k$  is the volume of the truncated uniform kernel under  $S_k(X)$ .

Given that we form the estimate  $\hat{f}_k$  at N points using M observations, the plug-in estimator is given by:

$$\hat{G}_k = \frac{1}{N} \sum_{i=1}^N g(\hat{f}_k(X_i), X_i)$$

where  $\hat{G}_k$  is identical to the standard kernel density estimator  $G_k'$  except for the volume—which in KDE is set to the untruncated value  $V_k(X) = k/M$ . It can be shown that the biases of the plug-in estimators  $\hat{G}_k, G_k'$  are given by

$$\mathbb{B}(\hat{G}_k) = \sum_{i=1}^d c_{1,i} \left(\frac{k}{M}\right)^{i/d} + \frac{c_2}{k} + o\left(\frac{1}{k}\right) + \frac{k}{M}$$

$$\mathbb{B}(G'_k) = c_1 \left(\frac{k}{M}\right)^{1/d} + \frac{c_2}{k} + o\left(\frac{1}{k} + \frac{k}{M}\right)$$

The variances of the plug-in estimators  $\hat{G}_k$ ,  $G'_k$  are identical up to leading terms and are given by

$$\mathbb{V}(\hat{G}_k) = \mathbb{V}(G_k') = c_4\left(\frac{1}{N}\right) + c_5\left(\frac{1}{M}\right) + o\left(\frac{1}{M} + \frac{1}{N}\right)$$

where  $c_4$  and  $c_5$  are constants that depend on g and f. We also need the extra assumptions that  $k\to\infty$  and  $k/M\to0$  to ensure that estimators are unbiased. We can see that as  $N\to\infty$  and  $M\to\infty$ , variance converges to 0.

To minimize the bias in both plugin estimators, the optimal choice of  $k = \Theta\left(M^{\frac{1}{1+d}}\right)$ , which gives us a bias

of  $\Theta\left(M^{\frac{-1}{1+d}}\right)$ . Since  $N, M \leq T$ , both KDE and truncated KDE have the assumed bias and variance rate necessary for the weighted estimator to achieve parametric MSE rate of convergence.

## 143 5.3 Minimax rate of entropy estimator

Without loss of generality, the analysis is restricted to functions supported by [0,1]. Define  $K=(K'_0,...,K'_m,K_0,...,K_m)$  for  $K'_i\leq K_i$  and  $0\leq i\leq m$ . Construct

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$$\mathcal{C}_m^i(K) = \{ f \in \mathcal{C}_m^i : K_i' \leq f^{(i)}(x) \leq K_i, \forall x \in [0,1], 0 \leq i \leq m \}$$

and also for  $0 < \nu \le 1$  and  $t, A \in \mathbb{R}_+$ , construct

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$$\mathcal{L}_{m+\nu}^{j}(K,A) = \{ f \in \mathcal{C}_{m}^{j}(K) : |f^{(m)}(y) - f^{(m)}(x)| \le A|y - x|^{\nu}, \forall x, y \in [0,1] \},$$
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$$\tilde{\mathcal{L}}_{m+\nu}(t,A) = \{ f \in \mathcal{L}_{m+\nu}^{\infty}(tU,A) : \int_{0}^{1} f(x) dx = 0 \}$$

- with  $U = \mathbf{1}_{m+1}$ ,  $\mathbf{1}_{m+1}$  where  $\mathbf{1}_{m+1}$  has all components equal to 1 in  $\mathbb{R}^{m+1}$ .
- We also make the following assumption
- Assumption  $\mathbb{A}(f,\mu)$ : There exist disjoint sets  $A_1,...,A_p$  and functions  $g_i$  satisfying the following relations for  $1 \le i \le p$ :
- 154 i.  $||g_i||_{\infty} \leq 1$ ;

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- 155 ii.  $||\mathbb{I}_{A_i} g_i||_1 = 0;$
- 156 iii.  $\int g_i(x) f(x) d\mu(x) = 0;$
- iv.  $\int g_i^2(x) f(x) d\mu(x) = a_i > 0$
- Theorem 1: Let  $\lambda = \{\lambda_1, \lambda_2, ..., \lambda_p\}$  where  $\lambda_i \in \Lambda = \{-1, 1\}^p$ . Define  $\bar{Q}_n = 2^{-p} \sum_{\lambda \in \Lambda} Q_{\lambda}^n$  and assuming  $\mathbb{A}(f, \mu)$  is satisfied. Also let

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$$\alpha = \sup_{1 \le i \le p} ||g_i||_{\infty}, \quad s = (n\alpha^2) \sup_{1 \le i \le p} P(A_i), \quad c = (n) \sup_{1 \le i \le p} a_i$$

Then, with  $C \leq \frac{1}{3}$ , we can upper bound the Hellinger distance by

$$h^{2}(P^{n}, \bar{Q}_{n}) \leq C(\alpha, s, c)n^{2} \sum_{i=1}^{p} a_{i}^{2}$$

The proof is lengthy and is omitted here. We can use this result and the Le Cam method to obtain the lower bound.

Corollary 1: Assume that T is a function defined on some subset  $\Theta$  of  $\mathbb{L}^1(\mu)$ , which contains f and some set of densities  $g_{\lambda}, \lambda \in \Lambda$ , derived from  $g_i$ 's which satisfy  $\mathbb{A}(f,\mu)$  with parameters  $\alpha,s,c$  as defined above. If (i)  $C(\alpha,s,c)n^2\sum_{j=1}^p\alpha_j^2\leq \gamma<1$  and (ii)  $\forall \lambda\in\Lambda, T(g_{\lambda})-T(f)\geq 2\beta>0$ , then for any estimator  $\hat{T}_n$  of T derived from n i.i.d. observations, we have for the joint distribution  $\mathbb{P}_g=g\cdot\mu$ 

$$\sup_{g \in \Theta} \mathbb{P}_g[|T(g) - \hat{T}_n| > \beta] \ge \frac{1}{2}[1 - (\gamma(2 - \gamma))^{1/2}]$$

170 *Proof:* Suppose T(f) = 0, define subsets  $\Theta_0$  and  $\Theta_1$  of  $\Theta$  as

$$\Theta_0 = \{g \in \Theta : T(g) \le 0\}, \qquad \Theta_1 = \{g \in \Theta : T(g) \ge 2\beta\}$$

By the Le Cam method, any test between  $\Theta_0$  and  $\Theta_1$  will have at least one of its errors as large as  $(1/2)[1 - (\gamma(2-\gamma))^{1/2}]$ . If we consider the particular test which accepts  $\Theta_0$  when  $\hat{T}_n \leq \beta$ , we get the same result as in

174 Corollary 1.

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To prove the lower bound in the multi-dimensional case, we will work on the hypercube  $H=[0,1]^d$  and consider functions in  $\tilde{L}_{m+\nu}(t,A)$ .

Theorem 2: Let f be some density in  $\Theta$  and  $\log f$  be bounded on H. Denote  $B_t$  as the set  $\{f+l|l\in \tilde{L}_{m+\nu}(t,A)\}$  where  $m,\nu,A$  are fixed constants and assume that  $B_t\subset\Theta$  for some small t and that when  $f+l\in B_t$ , we can expand

$$T(f+l) = T(f) + \int_H T'(x)l(x)dx + \frac{1}{2}\int_H T''(x)l^2(x)dx + ||l||_2^2 o(1)$$

where o(1) is a function of t and  $\inf_{x \in H} T''(x) > 0$ . Then

$$\lim_{t \to 0} \inf_{t \to 0} \inf_{\hat{T}_n} \inf_{g \in B_t} \mathbb{P}_g[|\hat{T}_n - T(g)| > \epsilon n^{-\gamma}] > 0$$

for some  $\epsilon > 0$  and  $\gamma = 4s/(4s+d)$ .

Proof: Divide the hypercube  $[0,1]^d$  into  $p=\prod_{i=1}^d p_i$  hyperrectangles with side lengths  $p_i^{-1}$  chosen in such a way that, for some K chosen later,  $K \leq A_i p_i^{-(m_i+\nu_i)} \leq 2K, 1 \leq i \leq d$ . On each hyperrectangles  $R_j, 1 \leq j \leq p$ , we can build a perturbation  $l_j$  such that for a fixed constant c,

$$\int_{R_j} l_j(x) dx = 0, \qquad \int_{R_j} T'(x) l_j(x) dx = 0, \qquad \int_{R_j} l_j^2(x) dx \ge \frac{c^2}{p}$$

188  $||D_i^{m_i}l_j||_{\infty} \leq p_i^m$  for  $1 \leq i \leq d$ . For  $\lambda \in \Lambda\{-1;1\}^p$ , setting

$$l_{\lambda}(x) = K \sum_{i=1}^{p} \lambda_{j} l_{j}(x) \mathbb{I}_{R_{j}}(x)$$

we see that for p large enough,  $f + l_{\lambda}$  belongs to  $\Theta$  for all  $\lambda$  and that

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$$T(f+l_{\lambda}) \geq T(f) + C_1 K^2$$

We can apply Corollary 1 with  $\sum_{j=1}^p \alpha_j^2 \le C_2 K^4/p$ . Since p is, by definition of K, of order  $K^{-d/s}$ , choosing  $K = C_3 n^{-2/(4+d/s)}$  gives us the desired result.

For the upper bound, we can construct an estimator  $\hat{f}$  of f based on r i.i.d. variables of density f such that for  $r \ge r_0$  not depending on f, the following holds:

196 i. 
$$\hat{f}\in\mathcal{C}^0_{2k}(K^\epsilon);$$

ii. for  $2 \ge q < \infty$  and  $0 \ge i \ge k$ ,

$$C_f(||\hat{f}^{(i)} - f^{(i)}||_q^q \le C_i'(q)r^{-q/6},$$

for some constants  $C'_i(q)$  that are independent of f.

Now we can define the estimator  $\hat{T}_n$  of T(f) as follows:

$$\hat{T}_n = T(\hat{f}) - \sum_{i=0}^k <\phi_i'(\hat{f},\hat{f}^{(i)}) > + \frac{1}{2}\sum_{i,j=0}^k <\phi_{i,j}''(\hat{f}),\hat{f}^{(i)}\hat{f}^{(j)} > + \overline{L(\hat{f})} + \frac{1}{2}\sum_{i,j=0}^k Q_{i,j}(\phi_{i,j}''(\hat{f}))$$

where  $\phi_1,...,\phi_q$  is an orthonormal system in  $\mathbb{L}^2([0,1],dx)$  which has the following properties:

- i.  $\phi_1 = 1$  and  $\phi_j(x) = 0$  for  $j \ge 2, x \notin [\epsilon, 1 \epsilon]$  for some  $\epsilon > 0$ ;
- ii. The linear space  $\mathbb{V}$  generated by  $\phi'_i$  is stable by differentiation.

Given this estimator, we can use the Taylor expansion and bounding the remainder to show that  $\mathbb{E}_f[|\hat{T}_n - T(f)|^2] \leq Cn^{-1}$ .

# 6 Conclusion

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In this paper, we have explored the theoretical foundations and performance in practice of an optimally weighted ensemble of slowly-converging entropy estimators. These estimators which have deteriorating MSE rates as the dimension d increases can be used in a weighted ensemble that can achieve the minimax  $O(T^{-1})$  rate of convergence. The weights can be determined by solving a convex optimization problem which does not require any training data. We also have shown that the popular kernel density estimator, its bias-corrected version, and the k-NN based Kozachenko-Leonenko estimator fit the conditions of having slow MSE rates of order  $O(T^{-\gamma/d})$  and can therefore be used to derive the weighted estimator.

Additionally, we ran some experiments to showcase the weighted ensemble estimator's superior performance 215 in approximating Shannon entropy compared to other widely-used entropy estimators and related the observed 216 results to our theoretical findings. Although we did not observe the same MSE rate when varying over the 217 dimension as [2] reported, we believe that the our experiment performed poorly when the dimension d > 8218 because the sample size of 3000 may not have been enough to estimate the Shannon entropy, and increasing 219 T should result in our estimators following the same trend as [2] observed. Assuming that the weighted 220 estimators can achieve the  $O(T^{-1})$  convergence rate as expected, the ensemble method poses as a promising 221 technique to perform effective entropy estimation. 222

In closing, entropy estimation is still an open area of research. One possible extension of the weighted estimator algorithm is to use an  $L_1$  norm instead of  $L_2$  to introduce sparsity. This approach may speed up the estimation process since there would be fewer estimators. Furthermore, we can apply the weighted ensemble to estimate other functionals of probability density that has a general form of  $\int \phi(f(x), f'(x), ..., f^{(k)}(x), x) dx$  such as divergence, mutual information, and intrinsic dimension.

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