Statistical Inference for Entropy

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1 Introduction

2 Entropies and Properties

Entropy can be thought of as a representation of the average information content of an observation; sometimes referred to as a measure of unpredictability or disorder.

2.1 Shannon Entropy

The Shannon entropy of a random vector X with density function f is given by;

$$H = -\mathbb{E}\{log(f(x))\} = -\int_{x:f(x)>0} f(x)log(f(x))dx \tag{1}$$

2.2 Rényi and Tsallis Entropy

These entropies are for the order $q \neq 1$ and the construction of them relies upon the generalisation of the Shannon entropy 1. For a random vector $X \in \mathbb{R}^d$ with density function f, we define;

Rényi entropy

$$H_q^* = \frac{1}{1-q} log\left(\int_{\mathbb{R}^d} f^q(x)dx\right) \qquad (q \neq 1) \tag{2}$$

Tsallis entropy

$$H_q = \frac{1}{q-1}\left(1 - \int_{\mathbb{R}^d} f^q(x)dx\right) \qquad (q \neq 1) \tag{3}$$

When the order of the entropy $q \to 1$, both the Renyi, (2), and Tsallis, (3), entropies tend to the Shannon entropy, (1).

3 Estimation of Entropy

3.1 Kozachenko-Leonenko Estimator

We now wish to introduce the Kozachenko-Leonenko estimator of the entropy H. Let $X_1, X_2, ..., X_n$, $N \geq 1$ be independent and identically distributed random vectors in $\mathbb{R}^d$, and denote $\|.\|$ the Euclidean norm on $\mathbb{R}^d$.

- For $i = 1, 2, ..., n$, let $X_{(1),i}, X_{(2),i}, .., X_{(n-1),i}$ denote an order of the X_k for $k = \{1, 2, ..., n\} \setminus \{i\}$, such that $\|X_{(1),i} - X_i\| \leq \cdots \leq \|X_{(n-1),i} - X_i\|$. Let the metric ρ, defined as;

$$\rho_{(k),i} = \|X_{(k),i} - X_i\| \tag{4}$$

denote the kth nearest neighbour or X_i.

- For dimension d, the volume of the unit d-dimensional Euclidean ball is defined as;

$$V_d = \frac{\pi^{\frac{d}{2}}}{\Gamma(1 + \frac{d}{2})} \tag{5}$$

- For the kth nearest neighbour, the digamma function is defined as;

$$\Psi(k) = -\gamma + \sum_{j=1}^{k-1} \frac{1}{j} \tag{6}$$

where $\gamma = 0.577216$ is the Euler-Mascheroni constant (where the digamma function is chosen so that $\frac{e^{\Psi(k)}}{k} \to 1$ as $k \to \infty$).

Then the Kozachenko-Leonenko estimator for entropy, H, is given by;

$$\hat{H}_n = \frac{1}{n} \sum_{i=1}^{n} log \left[\frac{\rho_{(k),i}^d V_d (n-1)}{e^{\Psi(k)}} \right] \tag{7}$$

This estimator for entropy, when $d \leq 3$, under a wide range of k and some regularity conditions, this estimator satisfies;

$$n\mathbb{E}(\hat{H}_n - H)^2 \to 0 \quad (n \to \infty) \tag{8}$$

so $\hat{H}_n$ is efficient in the sense that the asymptotic variance is the best attainable; $n^{\frac{1}{2}}(\hat{H}_n - H) \xrightarrow{d} N(0, Var[log(f(x))])$.

Later, I will further discuss this estimator for the specific dimensions $d = 1$ and $d = 2$; however, it is important to note that for larger dimensions this estimator is not accurate. When $d = 4$, equation 8 no longer holds but the estimator $\hat{H}_n$, defined by 7, is still root-n consistent, provided k is bounded. Also, when $d \geq 5$ there is a non trivial bias, regardless of the choice of k.

There is a new proposed estimator, formed as a weighted average of $\hat{H}_n$ for different values of k, explored in ... . Moreover, as this paper only considers $d = 1, 2$, this will not be examined here.

3.2 Bias of the K-L estimator

$\hat{H}_n$ is approximately an unbiased estimator for H; we wish to explore how approximate this is, by considering the bias of the estimator for entropy;

$$Bias(\hat{H}_n) = \mathbb{E}(\hat{H}_n) - H = \mathbb{E}(\hat{H}_n - H) \tag{9}$$

4 Monte-Carlo Simulations

In this section I will explore simulations of the bias of estimator (7) in comparison to the size of the sample estimated from, with respect to different values of k; firstly exploring 1-dimensional distributions and then progressing onto 2-dimensional.

I will begin by exploring entropy of samples from the normal distribution $N(0, \sigma^2)$, where without loss of generality we can use the mean $\mu = 0$ and change the variance σ^2 as needed. The normal distribution has an exact formula to work out the entropy, given the variance σ^2. Using equation (1) and the density function for the normal distribution $f(x) = \frac{1}{\sqrt{(2\pi)}\sigma} \exp\left(\frac{-x^2}{2\sigma^2}\right)$ for $x \in \mathbb{R}$, given $\mu = 0$, we can write the exact entropy for the normal distribution;

$$H = log(\sqrt{(2\pi e)}\sigma) \tag{10}$$

4.1 1-dimensional Normal Distribution