Estimation of Rényi Information Divergence via Pruned Minimal Spanning Trees[1]

Alfred Hero
Dept. of EECS,
The university of Michigan,
Ann Arbor, MI 48109-2122, USA
Email: hero@eecs.umich.edu

Olivier J.J. Michel
Laboratoire de Physique, URA-1325 CNRS,
École Normale Supérieure de Lyon,
46 allée d'Italie,
69364 Lyon Cedex 07, France
Email: omichel@physique.ens-lyon.fr

Abstract

In this paper we develop robust estimators of the Rényi information divergence (I-divergence) given a reference distribution and a random sample from an unknown distribution. Estimation is performed by constructing a minimal spanning tree (MST) passing through the random sample points and applying a change of measure which flattens the reference distribution. In a mixture model where the reference distribution is contaminated by an unknown noise distribution one can use these results to reject noise samples by implementing a greedy algorithm for pruning the k-longest branches of the MST, resulting in a tree called the k-MST. We illustrate this procedure in the context of density discrimination and robust clustering for a planar mixture model.

1. Introduction

Let $\mathcal{X}_n = \{x_1, x_2, \ldots, x_n\}$ denote a sample of i.i.d. data points in R^d having unknown Lebesgue multivariate density $f(x_i)$ supported on $[0,1]^d$. Define the order ν Rényi entropy of f [7]

$$H_\nu(f) = \frac{1}{1-\nu} \ln \int f^\nu(x)dx \qquad (1)$$

and, for a dominating Lebesgue density f_o, the Rényi information divergence of f with respect to f_o

$$I_\nu(f, f_o) = \frac{1}{1-\nu} \ln \int \left(\frac{f(x)}{f_o(x)}\right)^\nu f_o(x)dx \qquad (2)$$

The quantity $I_\nu(f, f_o)$ is a special case of I-divergence which is called the Chernoff distance or the Renyi cross-entropy between f and f_o [1]. The I-divergence takes on its minimum value (equals zero) if and only if $f = f_o$ (a.e.). The Rényi information divergence $I_\nu(f, f_o)$ specializes to the Rényi entropy $H_\nu(f)$ when f_o is equal to a uniform density over $[0,1]^d$. Other special cases of interest are obtained for $\nu = \frac{1}{2}$ for which one obtains the log Hellinger distance squared

$$I_{\frac{1}{2}}(f, f_o) = \ln \left(\int \sqrt{f(x) f_o(x)} dx \right)^2$$

and for $\nu \to 1$ for which one obtains the Kullback-Liebler divergence

$$\lim_{\nu \to 1} I_\nu(f, f_o) = \int f_o(x) \ln \frac{f_o(x)}{f(x)} dx.$$

The problem of estimating the I-divergence arises in the very large class of density classification problems for clustering and pattern recognition [1, 3]. In these problems one applies a threshold test to an estimate of $I_\nu(f, f_o)$ in order to decide whether f is equal to f_o. I-divergence estimation also arises in image registration where the I-divergence can be directly related to mutual information between two images f and f_o [8]. For an overview of entropy and I-divergence estimation applications the reader can refer to [2] and [1].

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In this paper we present a methodology robust estimation of $I_\nu(f, f_o)$ for unknown f and arbitrary dominating density f_o. This methodology performs a non-linear transformation on the data sample $\mathcal{X}_n$, producing a transformed data sample $\mathcal{Y}_n$, and constructs a graph, called the k-minimal spanning tree (k-MST), on a minimal k-point subset $\mathcal{Y}_{n,k}$ of the transformed data. The k-MST is a graph which connects k out of n of the data points in a manner that minimizes the total length of the graph, where length is defined as the sum of the interconnection distances (called edges) raised to a user-specified power $\gamma \in (0, d)$. This results in a strongly consistent and unbiased estimate of I_ν which has desirable properties including: the estimator does not require performing the difficult step of density estimation; estimates of various orders ν of I_ν can be obtained by varying teh edge power exponent; the sequence of trees $\mathcal{Y}_{n,2}, \ldots \mathcal{Y}_{n,n} = \mathcal{Y}_n$ provides a natural extension of rank order statistics for multidimensional data.

To illustrate our results we will show ROC curves for the MST estimates of Rényi information divergence and give an application to robust clustering for the case that f is a planar mixture density of the form

$$f = (1 - \epsilon) f_1 + \epsilon f_o, \tag{3}$$

where f_o is a known outlier density and $f_1, \epsilon \in [0, 1]$ are unknown.

2. MST's and Entropy Estimation

A spanning tree $\mathcal{T}$ through the sample $\mathcal{X}_n$ is a connected acyclic graph which passes through all the n points $\{x_i\}_i$ in the sample. $\mathcal{T}$ is specified by an ordered list of edge (Euclidean) lengths e_{ij} connecting certain pairs (x_i, x_j), $i \neq j$, along with a list of edge adjacency relations. The power weighted length of the tree $\mathcal{T}$ is the sum of all edge lengths raised to a power $\gamma \in (0, d)$, denoted by: $\sum_{e \in \mathcal{T}} |e|^\gamma$. The minimal spanning tree (MST) is the tree which has the minimal length $L(\mathcal{X}_n) = \min_{\mathcal{T}} \sum_{e \in \mathcal{T}} |e|^\gamma$. For any subset $\mathcal{X}_{n,k}$ of k points in $\mathcal{X}_n$ define $\mathcal{T}_{\mathcal{X}_{n,k}}$ the k-point MST which spans $\mathcal{X}_{n,k}$. The k-MST is defined as that k-point MST which has minimum length. Thus the k-MST spans a subset $\mathcal{X}^*_{n,k}$ defined by

$$L(\mathcal{X}^*_{n,k}) = \min_{\mathcal{X}_{n,k}} L(\mathcal{X}_{n,k})$$

The planar k-MST problem was shown to be NP-complete in [6]. Ravi *et al* proposed a greedy polynomial time algorithm for the planar k-MST problem with approximation ratio $O(k^{\frac{1}{4}})$.

Let $\nu \in (0, 1)$ be defined by $\nu = (d - \gamma)/d$ and define the statistic

$$\hat{H}_\nu(\mathcal{X}^*_{n,k}) = \frac{1}{1-\nu} \ln \left(n^{-\nu} L(\mathcal{X}^*_{n,k}) \right) + \beta(\nu, d) \tag{4}$$

where β is a constant equal to the Rényi antropy of the uniform density on $[0, 1]^d$. In [5] Hero and Michel presented a d-dimensional extension of the planar k-MST approximation of Ravi et al, called the greedy k-MST approximation. In that paper we proved that when $k = \alpha n$, $\alpha \in [0, 1]$, and the length $L(\mathcal{X}^*_{n,k})$ of this approximation is substituted into (4) one obtains a strongly consistent and robust estimator of the Rényi entropy (1):

$$\hat{H}_\nu(\mathcal{X}^*_{n,k}) \to \min_{A: P(A) \geq \alpha} \frac{1}{1-\nu} \ln \int_A f^\nu(x) dx \quad (a.s.)$$

where the minimization is performed over all d-dimensional Borel subsets of $[0, 1]^d$ having probability $P(A) = \int_A f(x) dx \geq \alpha$. This result was used in [4] to specify robust estimators of Rényi entropy which perform outlier rejection for the case that f is a mixture density of the form (3) with f_o uniform.

3. Extension: I-Divergence Estimation

Let $g(x)$ be a reference density on $\mathbf{R}^d$ which dominates the density $f(x)$ of a sample point $x = [x^1, \ldots, x^d]^T$ in the sense that for all x such that $g(x) = 0$ we have $f(x) = 0$. For any x such that $g(x) > 0$ let $g(x)$ have the product representation $g(x) = g(x^1) g(x^2|x^1) \ldots g(x^d|x^{d-1}, \ldots, x^1)$ where $g(x^k|x^{k-1}, \ldots, x^1)$ denotes the conditional density associated with $g(x)$ of the k-th component. In what follows we will ignore the set $\{x : g(x) = 0\}$ since, as $f(x) = 0$ over this set, it has probability zero. Now consider generating the vector $y = [y^1, \ldots, y^d]^T \in \mathbf{R}^d$ by the following vector transformation

$$\begin{aligned} y^1 &= G(x^1) \\ y^2 &= G(x^2|x^1) \\ &\vdots \\ y^d &= G(x^d|x^{d-1}, \ldots, x^1) \end{aligned} \tag{5}$$

where $G(x^k|x^{k-1}, \ldots, x^1) = \int_{-\infty}^{x^k} g(\tilde{x}^k|x^{k-1}, \ldots, x^1) d\tilde{x}^k$ is the cumulative conditional distribution of the k-th component, which is monotone increasing except on the zero probability set $\{x : g(x) = 0\}$. Thus, except for this probability zero set, the conditional distribution has an inverse $x^k = G^{-1}(y^k|x^{k-1}, \dots, x^1) = G^{-1}(y^k|y^{k-1}, \dots, y^1)$ and it can be shown (via the standard Jacobian formula for transformation of variables) that the induced joint density, $h(y)$, of the vector y takes the form:

$$h(y) = \frac{f(G^{-1}(y^1), \dots, G^{-1}(y^d|y^{d-1}, \dots, y^1))}{g(G^{-1}(y^1), \dots, G^{-1}(y^d|y^{d-1}, \dots, y^1))} \quad (6)$$

Let $L(\mathcal{Y}^*_{n,k})$ denote the length of the greedy approximation to the k-MST constructed on the transformed random variables y, where $\mathcal{Y}^*_{n,k}$ is the set of k points spanned by this k-MST approximation. Then, from the results of [5] cited in the previous section, we know that

$$\hat{H}_\nu(\mathcal{Y}^*_{n,k}) \to \frac{1}{1-\nu} \ln \int h^\nu(y) dy \quad (a.s.) \quad (7)$$

Making the inverse transformation $y \to x$ specified by (5) in the above integral, noting that, by the Jacobian formula, $dy = g(x)dx$, and using the expression (6) for h, it easy to see that the integral in the right hand side of (7) is equivalent to the Rényi information divergence of $f(x)$ with respect to $g(x)$

$$\frac{1}{1-\nu} \ln \int h^\nu(y) dy = \frac{1}{1-\nu} \ln \int \left(\frac{f(x)}{g(x)} \right)^\nu g(x) dx.$$

Hence we have established that $\hat{H}_\nu(\mathcal{Y}^*_{n,k})$ is a strongly consistent estimator of the Rényi information divergence above. The results of [5] can thus be easily be extended to classification against any *arbitrary* distribution f_o, and not just the uniform distribution studied in [4].

4. Applications

256 samples were simulated from a triangle-uniform mixture density $f = (1-\epsilon)f_1 + \epsilon f_0$ where $f_1(x) = (\frac{1}{2} - |x^1 - \frac{1}{2}|)(\frac{1}{2} - |x^2 - \frac{1}{2}|)$ is a (separable) triangular shaped product density and $f_0 = 1$ is a uniform density, both supported on the unit square $x = (x^1, x^2) \in [0,1]^2$. The Rényi information divergences $I(f, f_0)$ and $I(f, f_1)$ were estimated by $\hat{H}_\nu(\mathcal{X}_n)$ and $\hat{H}_\nu(\mathcal{Y}_n)$, respectively, for $\nu = \frac{1}{2}$ ($\gamma = 1$ in the k-MST construction). $\mathcal{Y}_n$ was obtained by applying the mapping $y = (y^1, y^2) = (F_1(x^1), F_1(x^2))$ to the data sample $\mathcal{X}_n$, where $F_1(u)$ is the marginal cumulative distribution function associated with the triangular density.

In a first sequence of experiments the estimates $\hat{H}_\nu(\mathcal{X}_n)$ and $\hat{H}_\nu(\mathcal{Y}_n)$ of the respective quantities $I(f, f_0)$ and $I(f, f_1)$ were thresholded to decide between the hypotheses $H_0 : \epsilon = 0$ vs. $H_1 : \epsilon \neq 0$ and $H_0 : \epsilon = 1$ vs. $H_1 : \epsilon \neq 1$, respectively. The receiver operating characteristic (ROC) curves are indicated in Figures 1 and 2. Note that, as expected, in each case the detection performance improves as the difference between the assumed H_0 and H_1 densities increases.

In a second sequence of experiments we selected two realizations of the triangle-uniform mixture model for the values $\epsilon = 0.1$ and $\epsilon = 0.9$. For the former case the triangular is the dominating density and for the latter case the uniform is the dominating density. In each case the k-MST was implemented ($k = 90$) as a robust clustering algorithm to identify data points from the dominating densities - in the former case the k-MST was applied directly to $\mathcal{X}_n$ while in the latter case it was applied to $\mathcal{Y}_n$. The resulting k-MST quantities $\hat{H}_\nu(\mathcal{X}_{n,k})$ and $\hat{H}_\nu(\mathcal{Y}_{n,k})$ can be interpreted as robust estimates of the uncontaminated Rényi information divergences $I(f_1, f_0)$ and $I(f_0, f_1)$. respectively. Figure 3-5 illustrate the effectiveness of these estimates as "outlier rejection" algorithms.

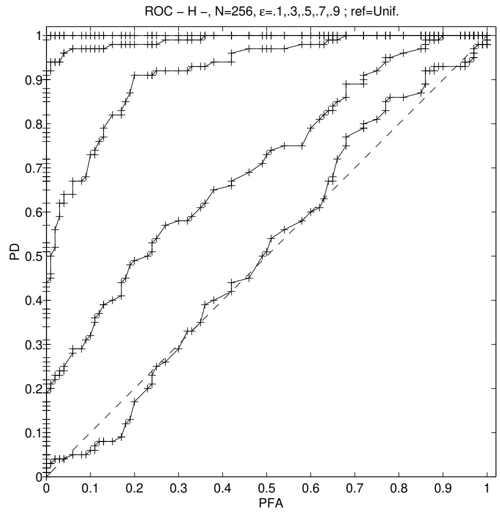

Figure 1. *ROC curves for the Rényi information divergence test for detecting triangle-uniform mixture density $f = (1-\epsilon)f_1 + \epsilon f_0$ (H_1) against the uniform hypothesis $f = f_0$ (H_0). Curves are decreasing in ϵ over the range $\epsilon \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$.*

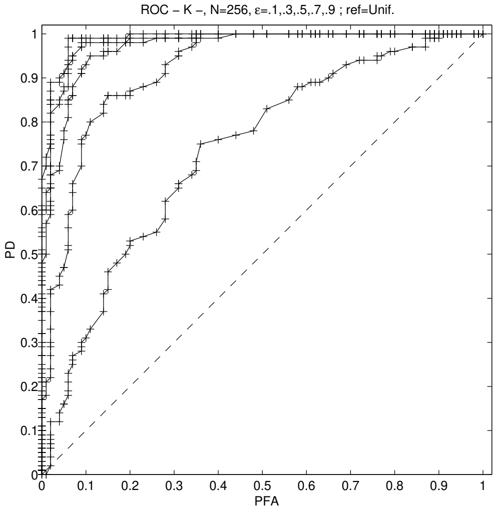

Figure 2. *Same as Figure 4 except test is against triangular hypothesis $f = f_1$ (H_0). Curves are increasing in ϵ.*

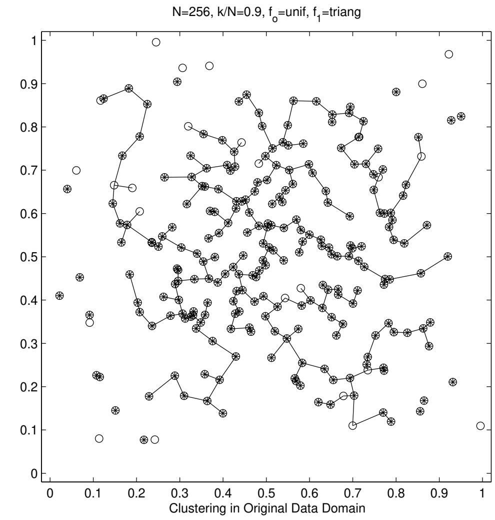

Figure 3. *A scatterplot of a 256 point sample from triangle-uniform mixture density with $\epsilon = 0.1$. Labels 'o' and '*' mark those realizations from the uniform and triangular densities, respectively. Superimposed is the k-MST implemented directly on the scatterplot $\mathcal{X}_n$ with $k = 230$.*

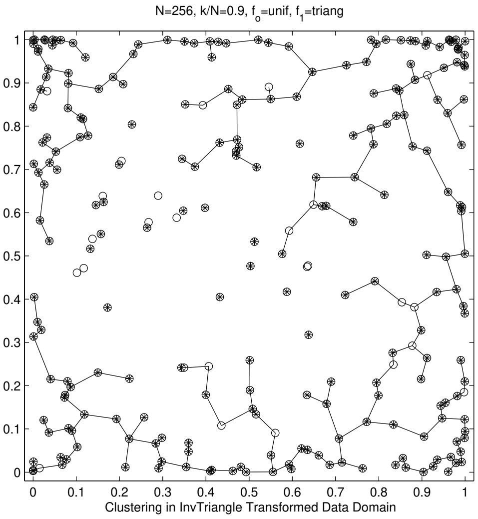

Figure 4. *A scatterplot of a 256 point sample from triangle-uniform mixture density with $\epsilon = 0.9$ in the transformed domain $\mathcal{Y}_n$. Labels 'o' and '*' mark those realizations from the triangular and uniform densities, respectively. Superimposed is the k-MST implemented on the transformed scatterplot $\mathcal{Y}_n$ with $k = 230$*

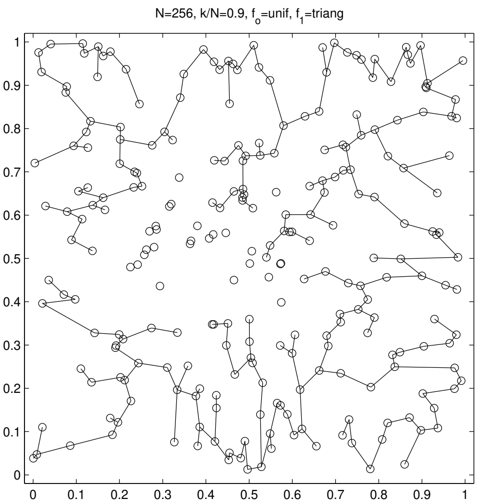

Figure 5. *Same as Figure 4 except displayed in the original data domain.*

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