kNN estimation of the unilateral dependency measure between random variables

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***Abstract*—The informational energy (IE) can be interpreted as a measure of average certainty. In previous work, we have introduced a non-parametric asymptotically unbiased and consistent estimator of the IE. Our method was based on the k^{th} nearest neighbor (kNN) method, and it can be applied to both continuous and discrete spaces, meaning that we can use it both in classification and regression algorithms. Based on the IE, we have introduced a unilateral dependency measure between random variables. In the present paper, we show how to estimate this unilateral dependency measure from an available sample set of discrete or continuous variables, using the kNN and the naïve histogram estimators. We experimentally compare the two estimators. Then, in a real-world application, we apply the kNN and the histogram estimators to approximate the unilateral dependency between random variables which describe the temperatures of sensors placed in a refrigerating room.**

I. Introduction

A critical aspect of many machine learning approaches is how well an information theory measure is estimated from the available training set. This relates to a standard concept in statistics – probability density estimation. *Density estimation* is the construction of an estimate of the density function from the observed data [1]. We will refer here only to *nonparametric estimation*, where less rigid assumptions will be made about the distribution of the observed data. Although it will be assumed that the distribution has the probability density f, the data will be allowed to speak for themselves in determining the estimate of f more than would be the case if f were constrained to fall in a given parametric family.

Much effort has been devoted to the nonparametric estimation of the mutual information (MI). The simplest approach is naïve estimation (which attempt to construct a histogram where every point is the center of a sampling interval) is plagued with both systematic (bias) and statistical errors [2]. An ideal estimator does not exist, and the choice of the estimator depends on the structure of data to be analyzed. It is not possible to design an estimator that minimizes both the bias and the variance to arbitrarily small values [2].

An alternative to the well-known MI measure is the unilateral dependency measure which can be derived from Onicescu's IE. Onicescu's IE was interpreted by several authors as a measure of expected commonness, a measure of average certainty, or as a measure of concentration. For a continuous random variable X with probability density function $f(x)$, the IE is [3], [4]:

$$IE(X) = \int_{-\infty}^{+\infty} f^2(x)dx \tag{1}$$

In order to study the interaction between two random variables X and Y, the following measure of unilateral dependency was defined by Andonie *et al.* [5]:

$$o(X,Y) = IE(X|Y) - IE(X) \tag{2}$$

with the following properties:

1) o is not a symmetric function;
2) $o(X,Y) \geq 0$ and the equality holds iff X and Y are independent;
3) $o(X,Y) \leq 1 - IE(X)$ and the equality holds iff X is completely dependent on Y.

This measure quantifies the unilateral dependence characterizing X with respect to Y and corresponds to the amount of information detained by Y about X. There is an obvious analogy between $o(X,Y)$ and the MI, since both measure the same phenomenon. However, the MI is a symmetric, not a unilateral measure.

When studying the interaction between two random variable, why is a unilateral dependency measure useful, and why do we not simply use the well-known MI? Let us consider two sets of experiments, characterized respectively by random variables X and Y. The experiments run simultaneously and interact probabilistically. Our question is which variable influences probabilistically more the other one. Thus, X can be viewed as $X|Y$ and Y can be viewed as $Y|X$. While the correlation quantifies linear dependency and MI describes the degree of interdependence between two random variables, the asymmetric measure $o(X,Y)$ helps us understand which random variable, X or Y, has a higher influence on the

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other one. If both X and $X|Y$ are available, we can estimate $IE(X|Y)$ as well as $o(X,Y)$, and similarly for Y and $Y|X$.

When the data is acquired from real world experiments or from simulators, we need to store series of values for X and Y featuring the two phenomena running independently, as well as measurements of values generated by the two phenomena running simultaneously, in order to capture $X|Y$ and $Y|X$. Moreover, the precision of the $IE(X|Y)$ and $o(X,Y)$ estimators increase when more values of $X|Y$ are available for each value of Y.

In the present paper, we introduce two statistical inference techniques for the unilateral dependency measure $o(X,Y)$ using *a.)* the kNN estimation method, and *b.)* the naïve histogram estimation. Based on a simple probability distribution, we experimentally compare the two estimators. Then, in a real-world application, we apply the histogram and the kNN estimators to approximate the unilateral dependency between random variables which describe the temperatures of sensors placed in a refrigerating room with.

The rest of the paper is structured as follows. Section II gives an overview of previous work. Section III briefly describes the kNN IE approximation method. In Section IV we introduce our new kNN approximator for the $o(X,Y)$ measure. In Section V, we describe how we adapt the naïve histogram method, a standard technique, for the $o(X,Y)$ estimation. Section VI compares the kNN and histogram $o(X,Y)$ estimators. We conclude in Section VII with a synthetic comparison of the two introduced estimators.

II. Previous work

In a sequence of papers ([6], [7], [8], [9]), we have introduced a Parzen windows approach for the approximation of the $o(X,Y)$ dependency measure from sample datasets. We used this approach in classification and feature weighting, in combination with LVQ and Neural Gas type algorithms. The Parzen windows estimate cannot be applied on continuous spaces, and this is an important drawback. This means that the Parzen windows estimation of $o(X,Y)$ cannot be applied in an important machine learning domain – continuous function approximation (or prediction). We note that the same inconvenience exists when estimating the Shannon type MI through Parzen windows.

To overcome this problem, our first step was to introduce a kNN estimator for the IE in [10]. We proved that this estimator is asymptotically unbiased and consistent [11] (i.e., it is a "good" estimator). Let us remind ourselves that a statistic whose mathematical expectation is equal to its intended parameter is called *unbiased* estimator of that parameter. Otherwise, the statistic is said to be *biased*. A statistic that converges asymptotically to its intended parameter, as its sample size increases, is called *consistent* estimator of that parameter [12].

In accordance to our results from [11], we can state now that the kNN is a "good" $o(X,Y)$ estimator, both for the discrete and the continuous case.

III. k^{TH} nearest neighbor estimation of the Informational Energy

From our previous results [10], [11], we will summarize how we can estimate $IE(X)$ from a random sample x_1, x_2, ..., x_n of d-dimensional observations, with a distribution having the unknown probability density $f(x)$.

The kNN estimators represent an attempt to adapt the amount of smoothing to the "local" density of data. The degree of smoothing is controlled by an integer k, chosen to be considerably smaller than the sample size. Let us denote $d_j(x_i)$ the distance from the reference point x_j to the point x_i. For each x_i, we define $d_1(x_i) \leq d_2(x_i) \leq \ldots \leq d_n(x_i)$ to be the distances from x_i to all other points of the sample, arranged in ascending order.

The kNN density estimate of probability density function $f(x)$ in x_i is defined by [1]:

$$\hat{f}(x_i) = \frac{k}{2nd_k(x_i)} \tag{3}$$

The IE is the average of the $f(x)$ values, as can be seen from eq. (1), that is $IE(X) = E(f(x))$. Since all n observations from our samples have the same probability $1/n$, a convenient estimator for IE is:

$$\hat{IE}_k^{(n)}(X) = \frac{1}{n}\sum_{i=1}^{n}\hat{f}(x_i) \tag{4}$$

where $\hat{f}(x_i)$ is the estimate of the probability density function $f(x_i)$.

To evaluate this formula, we have to obtain $\hat{f}(x_i)$. We start by determining the probability density $P_{ik}(\epsilon)$ of the random distance $R_{i,k,n}$ between a fixed point x_i and its k^{th} nearest neighbor, selected from the remaining $n-1$ points. The probability $P_{ik}(\epsilon)d\epsilon$ of the k^{th} nearest neighbor, to be within distance $R_{i,k,n} \in [\epsilon, \epsilon + d\epsilon]$ from x_i, can be expressed in terms of the trinomial formula [13]:

$$P_{ik}(\epsilon)d\epsilon = \frac{(n-1)!}{1!(k-1)!(n-k-1)!}dp_i(\epsilon)p_i^{k-1}(1-p_i)^{n-k-1}$$

where $p_i(\epsilon) = \int_{\|x-x_i\|<\epsilon} f(x)dx$ is the mass of the ϵ-ball centered at x_i and $\int P_{ik}(\epsilon)d\epsilon = 1$. We notice here that the distance between x_i and a subset of $k-1$ points is smaller than ϵ, while the distance to the remaining $n-k-1$ points is larger than $\epsilon + d\epsilon$.

We can express the expected value of $p_i(\epsilon)$ using the probability mass function of the trinomial distribution:

$$E_{P_{ik}(\epsilon)}(p_i(\epsilon)) = \int_0^\infty P_{ik}(\epsilon)p_i(\epsilon)d\epsilon =$$

$$= k\binom{n-1}{k}\int_0^1 p^{k-1}(1-p)^{n-k-1}pdp =$$

$$= k\binom{n-1}{k}\int_0^1 p^{(k+1)-1}(1-p)^{(n-k)-1}dp.$$

This equality can be reformulated using the *Beta* function:

$$B(m,n) = \int_0^1 x^{m-1}(1-x)^{n-1}dx = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}.$$

We obtain:

$$E_{P_{ik}(\epsilon)}(p_i(\epsilon)) = k\binom{n-1}{k}\frac{\Gamma(k+1)\Gamma(n-k)}{\Gamma(n+1)} =$$

$$= k\frac{(n-1)!}{(n-k-1)!k!}\frac{k!(n-k-1)!}{n!},$$

which can be rewritten as:

$$E_{P_{ik}(\epsilon)}(p_i(\epsilon)) = \frac{k}{n}. \tag{5}$$

On the other hand, assuming that $f(x)$ is almost constant in the entire ϵ-ball around x_i, we have [13]:

$$p_i(\epsilon) \approx V_1 R_{i,k,n}^d f(x_i)$$

where we denote the volume of the ball of radius $\rho_{r,n}$ in a d-dimensional space by

$$V_{\rho_{r,n}} = V_1 \rho_{r,n}^d = \frac{\pi^{\frac{p}{2}}\rho_{r,n}^d}{\Gamma(\frac{p}{2}+1)}.$$

V_1 is the volume of the unit ball and $R_{i,k,n}$ is the Euclidean distance between the reference point x_i and its k^{th} nearest neighbor. This means that $V_1 R_{i,k,n}^d$ is the volume of the d-dimensional ball of radius $R_{i,k,n}$. By using the Euclidean distance, we assume that all dimensions are at the same scale.

We obtain the expected value of $p_i(\epsilon)$:

$$E(p_i(\epsilon)) = E(V_1 R_{i,k,n}^d f(x_i)) = V_1 R_{i,k,n}^d \hat{f}(x_i). \tag{6}$$

Equations (5) and (6) both estimate $E(p_i(\epsilon))$. Their results are approximatively equal:

$$V_1 R_{i,k,n}^d \hat{f}(x_i) = \frac{k}{n}.$$

That is:

$$\hat{f}(x_i) = \frac{k}{nV_1 R_{i,k,n}^d}, i = 1 \dots n. \tag{7}$$

This is the estimated probability density function. By substituting $\hat{f}(x_i)$ in eq. (4), we finally obtain the following IE approximation:

$$\widehat{IE}_k^{(n)}(X) = \frac{1}{n}\sum_{i=1}^{n}\frac{k}{nV_1 R_{i,k,n}^d}. \tag{8}$$

According to [11], $\widehat{IE}_k^{(n)}(X)$ is asymptotically unbiased and consistent (i.e., it is a "good" estimator).

IV. The kNN $o(X,Y)$ estimator

Our goal is to infer $o(X,Y)$ from the random sample x_1, x_2, …, x_n. We will use the results from Section III to deduct a new kNN estimator for $o(X,Y)$.

First, we substitute $\widehat{IE}_k^{(n)}(X)$ from eq. (8) in eq. (2):

$$\hat{o}(X,Y) = \widehat{IE}_k^{(n)}(X|Y) - \widehat{IE}_k^{(n)}(X) \tag{9}$$

where:

$$\widehat{IE}_k^{(n)}(X|Y) = \sum_{j=1}^{m}\hat{f}(y_j)\widehat{IE}_k^{(n)}(X|y_j) \tag{10}$$

and

$$\widehat{IE}_k^{(n)}(X) = \frac{1}{n}\sum_{i=1}^{n}\frac{k}{nV_1 R_i^d} \tag{11}$$

is an adaptation of eq. (8).

We can write:

$$\widehat{IE}_k^{(n)}(X|y_j) = \frac{1}{n}\sum_{i=1}^{n}\hat{f}(x_i|y_j)$$

where

$$\hat{f}(x_i|y_j) = \frac{\hat{f}(x_i,y_j)}{\hat{f}(y_j)}. \tag{12}$$

We re-write the right hand side of this equation by using the estimated probability density function from eq. (7):

$$\hat{f}(x_i,y_j) = \frac{k_{ij}}{mnV_1 R_{i,j}^d}, i = 1 \dots n, j = 1 \dots m$$

$$\hat{f}(y_j) = \frac{k_j}{mV_1 R_j^d}, j = 1 \dots m$$

and we obtain:

$$\hat{f}(x_i|y_j) = \frac{k_{ij}}{mnV_1 R_{i,j}^d}\frac{mV_1 R_j^d}{k_j} = \frac{k_{ij}R_j^d}{nk_j R_{i,j}^d}.$$

R_i is the Euclidean distance between the reference point x_i and its k_i^{th} nearest neighbor, when the points are drawn from the one-dimensional probability distribution $f(x)$: $R_i = \|x_i - x_{i,k_i}\|$. Similarly, R_j is the Euclidean distance between the reference point y_j and its k_j^{th} nearest neighbor, when the points are drawn from the one-dimensional probability distribution $f(Y)$: $R_j = \|y_j - y_{j,k_j}\|$. Then, R_{ij} is the Euclidean distance between the reference point (x_i, y_j) and its k_{ij}^{th} nearest neighbor, when the points are drawn from the joint probability distribution $f(X,Y)$: $R_{ij} = \sqrt{(x_{ij} - x_{ij,k_{ij}})^2 + (y_{ij} - y_{ij,k_{ij}})^2}$.

Now we can re-write eq. (10):

$$\widehat{IE}_k^{(n)}(X|Y) = \sum_{j=1}^{m}\hat{f}(y_j)\frac{1}{n}\sum_{i=1}^{n}\frac{k_{ij}R_j^d}{nk_j R_{i,j}^d}$$

and the estimate of $o(X,Y)$ is:

$$\hat{o}(X,Y) = \sum_{j=1}^{m} \frac{k_j}{mV_1 R_j^d} \frac{1}{n} \sum_{i=1}^{n} \frac{k_{ij} R_j^d}{n k_j R_{i,j}^d} - \frac{1}{n} \sum_{i=1}^{n} \frac{k_i}{nV_1 R_i^d}$$

Therefore:

$$\hat{o}(X,Y) = \frac{1}{n^2 V_1} \left(\frac{1}{m} \sum_{j=1}^{m} \sum_{i=1}^{n} \frac{k_{ij}}{R_{i,j}^d} - \sum_{i=1}^{n} \frac{k_i}{R_i^d} \right) \tag{13}$$

We may think to simplify this expression by setting $k_i = k_{ij}$, and obtaining:

$$\hat{f}(x_i|y_j) = \frac{R_j^d}{n R_{i,j}^d},$$

but this is not always a good option. However, although we do not have a general method to set the nearest neighbor parameter, Silverman [1] suggests that an optimal choice of k is proportional to

$$n^{4/(d+4)}. \tag{14}$$

In our case, the optimal values of k_i and k_{ij} may not be equal, because these two parameters refer to different samples.

V. Histogram estimation of $o(X,Y)$

The naïve histogram estimation of a probability density function is a standard technique (see [1]). We will show how we can use it for inferring $o(X,Y)$, and this method will be an alternative to our kNN estimator from Section IV.

Considering the same random sample x_1, x_2, ..., x_n as above, the histogram estimator of probability density function $f(x)$ in x_i is:

$$\hat{f}(x_i) = \frac{\text{number of } x \text{ falling in the same bin as } x_i}{nh} \tag{15}$$

where n is the sample size and h is the bin width. All points falling in the same bin have the same $\hat{f}(x)$. The empirical value of IE can be written as:

$$IE_{\text{empirical}}(X) = \frac{\sum_{i=1}^{n} \hat{f}(x_i)}{n}. \tag{16}$$

From eqs. (15) and (16), the estimate of the IE can be expressed by

$$IE_{\text{empirical}}(X) = \frac{\sum_{\text{bin}=1}^{\text{number of bins}} (n_{\text{bin}})^2}{n^2 h} \tag{17}$$

where n_{bin} is the number of points in the current bin. We add in each bin n_{bin} times the number n_{bin} of points falling into the same bin as x_i.

In the case of the conditional probability density function, we draw for each point y several points x_y from $f(x|y)$, and find $IE_{\text{empirical}}(X|Y)$ by a formula similar to eq. (17).

The empirical value of $o(X,Y)$, obtained from the histogram is:

$$o_{\text{empirical}}(X,Y) = IE_{\text{empirical}}(X|Y) - IE_{\text{empirical}}(X).$$

VI. Experiments

A. A simple probability distribution

The non-parametric estimation of the IE is appropriate when the available sample has an unknown distribution. Nevertheless, it is interesting to compare the estimator's outcome with the results provided by a wider used technique, such as the naïve histogram estimation, as well as with the theoretical value of a probability density function.

In our experiments, we consider the joint probability density function

$$f_{X,Y}(x,y) = \frac{6}{5}\left(x + y^2\right), x \in [0,1], y \in [0,1], \tag{18}$$

which has the marginal probability density functions

$$f_X(x) = \int_0^1 \frac{6}{5}\left(x + y^2\right) dy = \frac{6}{5}\left(x + \frac{1}{3}\right)$$

and

$$f_Y(y) = \int_0^1 \frac{6}{5}\left(x + y^2\right) dx = \frac{6}{5}\left(\frac{1}{2} + y^2\right).$$

The conditional probability density function is:

$$f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)} = \frac{x + y^2}{\frac{1}{2} + y^2},$$

and the theoretical value of $o(X,Y)$ is:

$$o(X,Y) = IE(X|Y) - IE(X)$$

$$IE(X) = \int_0^1 f^2(x)dx = 1.12$$

$$IE(X|Y) = \int_0^1 \int_0^1 f_{X,Y}(x,y) f_{X|Y}(x|y) dxdy = 1.1351$$

and

$$o(X,Y) = 1.1351 - 1.12 = 0.0151.$$

A similar method can be used to find the values $IE(Y) = 1.128$, $IE(Y|X) = 1.14787$, and $o(Y,X) = 0.01987$.

To compare the theoretical values with the kNN and the histogram estimates, we need a sample of values drawn from the proposed distribution. The rejection sampling method [14] is appropriate for our case because we can find the inverses of the $f(x)$, $f(y)$ and $f(x|y)$ functions.

We draw a value from $f_X(x)$ by finding first the cumulative density function

$$F(x) = \int_0^x \frac{6}{5}\left(z + \frac{1}{3}\right) dz = \frac{3x^2 + 2x}{5}$$

and then its inverse

$$x = F^{-1}(t) = \frac{\sqrt{15t + 1} - 1}{3}$$

where t is a uniform random number from $[0,1]$.

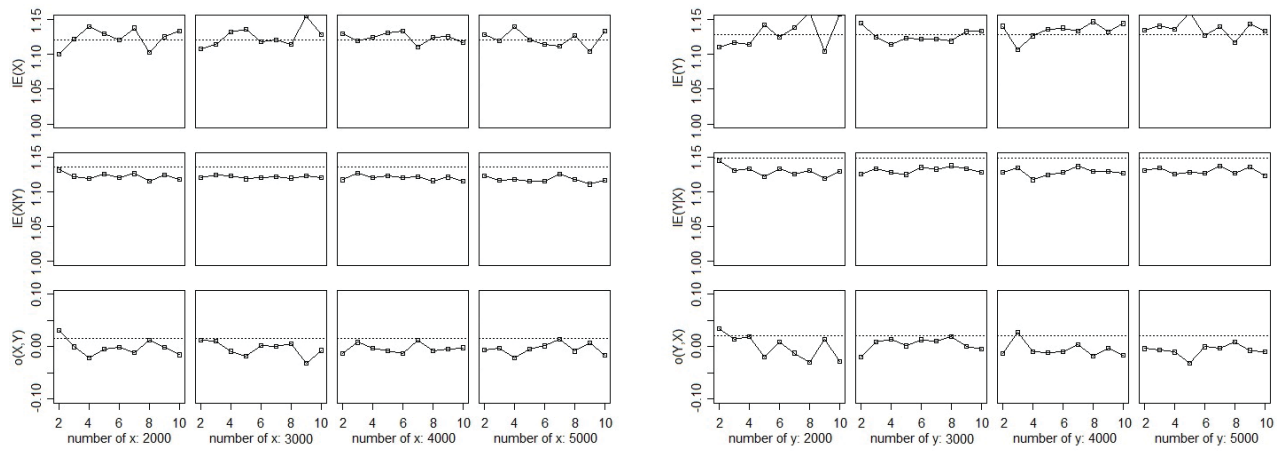


Fig. 1. The empirical value of $o(X,Y)$ determined from the histogram, with bin width of 15 points. The theoretical values $IE(X) = 1.12$, $IE(X|Y) = 1.1351$, $o(X,Y) = 0.0151$, $IE(Y) = 1.128$, $IE(Y|X) = 1.14787$, $o(Y,X) = 0.01987$ have been marked with dashed lines.

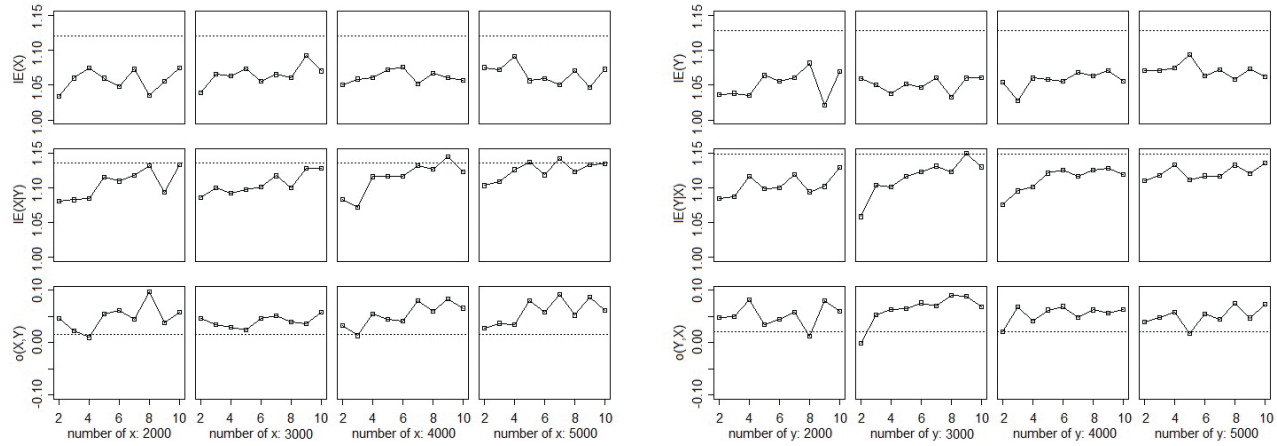


Fig. 2. The kNN estimated value of $o(X,Y)$, where k was determined with formula (14). The theoretical values $IE(X) = 1.12$, $IE(X|Y) = 1.1351$, $o(X,Y) = 0.0151$, $IE(Y) = 1.128$, $IE(Y|X) = 1.14787$, $o(Y,X) = 0.01987$ have been marked with dashed lines. $IE(X|Y)$ and $IE(Y|X)$ converge towards the theoretical values when the number of samples increase.

A sample from $f_{X|Y}(x|y)$ can be drawn with a two steps method. First, we draw a sample y from $f_Y(y)$. Next, we have to determine the cumulative density function of $f_{X|Y}(x|y)$:

$$F(x|y) = \int_0^x \frac{z+y^2}{\frac{1}{2}+y^2} dz = \frac{x^2+2xy^2}{1+2y^2}$$

and

$$x_y = F^{-1}(w) = -y^2 + \sqrt{2wy^2 + +y^4}$$

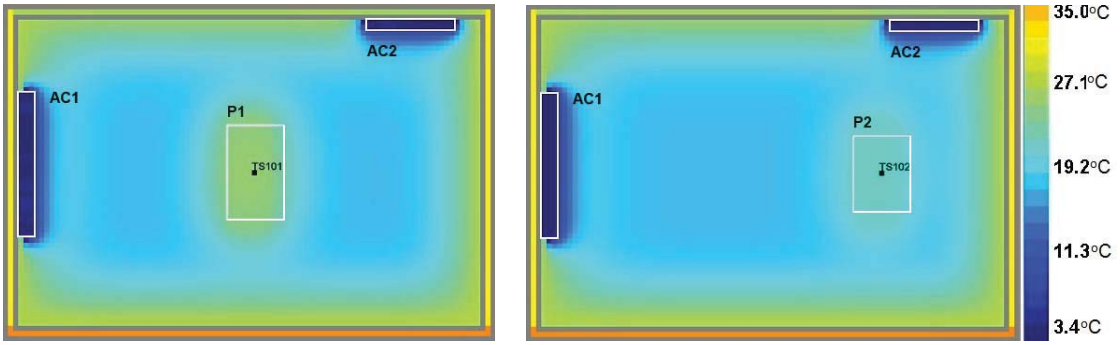
where w is a uniform random number from $[0,1]$ and y is the sample determined at the first step.

For a better fit with the theoretical conditional probability distribution function $f_{X|Y}(x|y)$, we generate between 2–10 x values for each y value, and between 2000–5000 y points. We apply the histogram method for 15 points in each bin because we determined experimentally that this value provided the most accurate estimations for our example. The kNN estimator is tested with the values of k_i and k_{ij} determined directly by formula (14), without applying any scale.

The histogram estimation (Fig. 1) looks unbiased, but has a large variability around the true values, even when the data sample size increases. Moreover, the estimated value of $o(X,Y)$ is mostly negative although it should be positive, as known from its properties. The kNN estimation (Fig. 2) is biased and tends to underestimate the true values. However, when the data sample size increases, the kNN estimation becomes more accurate, because it is asymptotically unbiased and consistent.

B. Temperature sensors data

In our real-world application, we study the temperature drop of two parcels placed in a room which is refrigerated by two air conditioning units $AC1$ and $AC2$. The experimental data are obtained with the emulator introduced in [15]. Each of the two air conditioners generate a temperature of 1°C. The two parcels *P1* and *P2* at initial temperatures 25°C and 20°C, having the sensors *TS101* and *TS102* attached, are placed in the room at various positions. We study the temperature variation



(a) Scenario *S1* (b) Scenario *S2*

(c) Scenario *S3.1* (d) Scenario *S4.1*

Fig. 3. Sample scenarios running on the data obtained with the emulator presented in [15]. The sensors *TS101* and *TS102* measure the temperatures of the parcels *P1* and *P2*. The low temperature produced by the air conditioning units $AC1$ and $AC2$ spread across the room as figured out by the image colors.

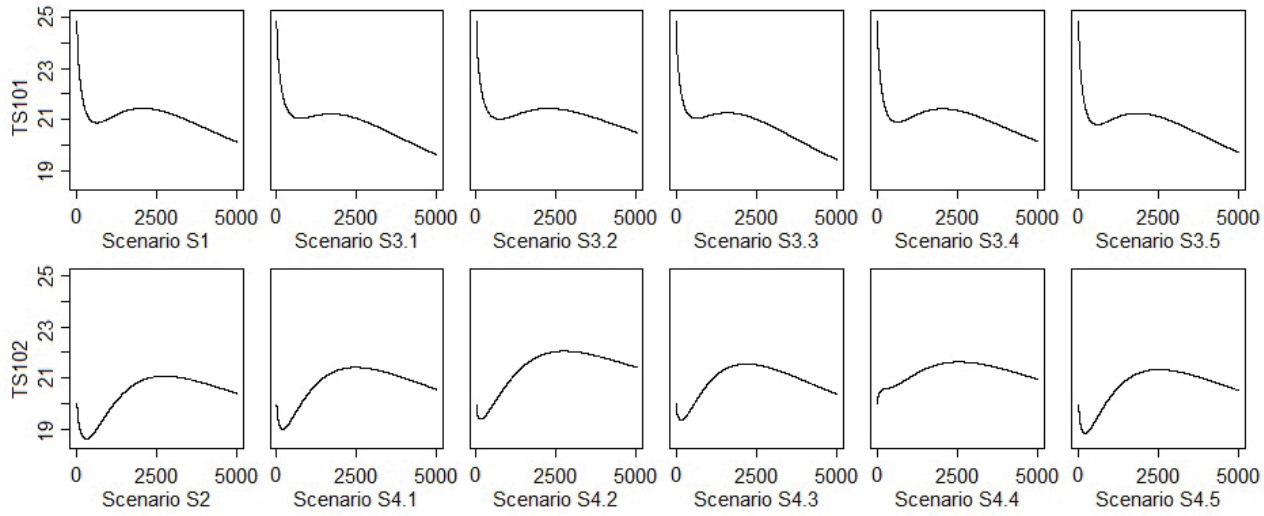


Fig. 4. The temperature values recorded in the mentioned scenarios along of 5000 ticks.

recorded by *TS101* and *TS102* under the following scenarios:

S1. Parcel *P1* is placed at position *POS1* to obtain the values of X measured by sensor *TS101*.

S2. Parcel *P2* is placed at position *POS2* to obtain the values of Y measured by sensor *TS102*.

S3. Parcel *P1* is placed at position *POS1*. The parcel *P2* is also placed, but its position slightly varies around *POS2*. For each new position of parcel *P2*, we measure a new series of values $X|Y$ from the *TS101* sensor.

S4. Parcel *P2* is placed at position *POS2*. The parcel *P1* is also placed, but its position slightly varies around *POS1*. For each new position of parcel *P1*, we measure a new series of values $Y|X$ via the sensor *TS102*.

These experiments allow us to determine how the presence of a parcel in the neighborhood of the other affects the evolution of temperatures recorded by the two sensors. We

TABLE I
HISTOGRAM ESTIMATION WITH 5 BINS.

Data / scenario	*TS101*			Data / scenario	*TS102*		
	$IE(X)$	$IE(X\|Y)$	$o(X,Y)$		$IE(Y)$	$IE(Y\|X)$	$o(Y,X)$
S1, *S3.1*	0.4973212	0.4647864	-0.032534	*S4*, *S4.1*	0.7889546	0.776226	-0.012728
S1, *S3.1*, *S3.2*	0.4973212	0.5695512	0.0722299	*S4*, *S4.1*, *S4.2*	0.7889546	0.4582482	-0.330706
S1, *S3.1*, ..., *S3.3*	0.4973212	0.5428637	0.0455425	*S4*, *S4.1*, ..., *S4.3*	0.7889546	0.4442722	-0.344682
S1, *S3.1*, ..., *S3.4*	0.4973212	0.5634884	0.0661671	*S4*, *S4.1*, ..., *S4.4*	0.7889546	0.481437	-0.307517
S1, *S3.1*, ..., *S3.5*	0.4973212	0.5471003	0.0497791	*S4*, *S4.1*, ..., *S4.5*	0.7889546	0.4640422	-0.324912

TABLE II
KNN ESTIMATION.

Data / scenario	*TS101*			Parameters		Data / scenario	*TS102*			Parameters	
	$IE(X)$	$IE(X\|Y)$	$o(X,Y)$	k_i	k_{ij}		$IE(Y)$	$IE(Y\|X)$	$o(Y,X)$	k_j	k_{ji}
S1, *S3.1*	0.9104424	1.678031	0.7675881	909	292	*S4*, *S4.1*	0.9096563	3.382819	2.473163	909	292
S1, *S3.1*, *S3.2*	0.9104424	1.226694	0.3162511	909	463	*S4*, *S4.1*, *S4.2*	0.9096563	1.064047	0.1543904	909	463
S1, *S3.1*, ..., *S3.3*	0.9104424	1.07795	0.1675078	909	607	*S4*, *S4.1*, ..., *S4.3*	0.9096563	1.180015	0.2703589	909	607
S1, *S3.1*, ..., *S3.4*	0.9104424	1.010859	0.1004169	909	736	*S4*, *S4.1*, ..., *S4.4*	0.9096563	1.157799	0.2481422	909	736
S1, *S3.1*, ..., *S3.5*	0.9104424	0.9918889	0.0814465	909	854	*S4*, *S4.1*, ..., *S4.5*	0.9096563	0.9812464	0.0715900	909	854

randomly re-position the parcels *P1* and *P2* five times each, denoting these scenarios by *S3.1–S3.5* and *S4.1–S4.5*. The emulated scenarios *S1*, *S2*, *S3.1*, and *S4.1* are presented in Fig. 3. The temperatures recorded in the above mentioned scenarios after 5000 ticks are depicted in Fig. 4. From the simulation of scenarios *S1* and *S2*, we obtain the samples of random variables X and Y. For each value of X, we obtain one corresponding value of $X|Y$ from scenario *S3.1*. For additional precision, for each value of X, we can obtain a set of values of $X|Y$ if we run the scenarios *S3.1 – S3.5*. The same idea applies for Y and $Y|X$.

Table I summarizes the experimental results obtained with the histogram estimator. The histogram method yields nearly constant values for $IE(X|Y)$ and $IE(Y|X)$, given a fixed number of bins, meaning that increasing the data set has little impact on this estimator. Nevertheless, the values of $o(X,Y)$ and $o(Y,X)$ should be positive, thus the bias is an important element in this case.

Table II summarizes the experimental results obtained with the kNN estimator. The kNN estimator of the IE becomes more precise when the volume of the available data increases. Thus, we progressively increase the amount of experimental data, starting with the data measured in scenarios *S1* and *S3.1*, and ending with the data measured in scenarios *S1*, *S3.1*, ..., *S3.5* for $IE(X|Y)$, and similarly with scenarios *S2* and *S4* for $IE(Y|X)$. The decrease of $IE(X|Y)$ is more robust when the formula (14) is used to set parameters k_i, k_{ij}, k_j and k_{ji}. We notice that it is important to adapt the values of these parameters to the sample size, in order to avoid the limitation of the k^{th} nearest distance. Overall, $IE(Y|X)$ also decreases, but not as clear as $IE(X|Y)$, meaning that Y is more sensitive to external influences. We can say that X has a stronger influence on Y than Y on X, which might lead to the decision to remove the sensor *TS102* because its information appears to be less relevant.

VII. CONCLUSIONS

In our examples, summarized in Figs. 1 and 2, all with unidimensional variables, histogram estimation is computationally more efficient than the kNN method and is more stable than the kNN estimator (smaller variance and smaller bias). However, for data sets with two or more dimensions, the histogram method becomes computationally expensive, due to the rapid increase of the number of bins. Another known drawback of the histogram method is the bias generated by the origin and width of the bins have a strong influence. It is difficult to find optimal values for the parameters of the bins (i.e., their hyper-volume, origin, and orientation) [1].

It is true, the kNN estimator is computationally more intensive than the histogram method (at least for unidimensional variables), but it is a "good" estimator – it is asymptotically unbiased and consistent – which are nice properties that the histogram method lacks. Therefore, it is generally more accurate than the histogram estimator.

The histogram method may be used, for instance, to process in real time a data stream, and draw a quick (but not final) conclusion. The kNN method is perhaps more useful in batch mode, as a second step, to consolidate the results.

Approximating $o(X,Y)$ from from sample datasets becomes more relevant if this measure is incorporated into machine learning algorithms, as we did in [6], [7], [8], and [9]. In classification algorithms, all three estimators (Parzen windows, kNN, and histogram) may be used to approximate $o(X,Y)$ from data samples. In the future, it may be interesting to compare their relative performances. For continuous function approximation, only the kNN and the histogram methods may be used.

REFERENCES

[1] B. Silverman, *Density Estimation for Statistics and Data Analysis (Chapman & Hall/CRC Monographs on Statistics & Applied Probability)*. Chapman and Hall/CRC, 1986.

[2] J. A. Bonachela, H. Hinrichsen, and M. A. Munoz, "Entropy estimates of small data sets," *Journal of Physics A: Mathematical and Theoretical*, vol. 41, p. 202001, 2008.

[3] O. Onicescu, "Theorie de l'information. energie informationelle," *C. R. Acad. Sci. Paris, Ser. A–B*, no. 263, pp. 841–842, 1966.

[4] S. Guiasu, *Information theory with applications*. McGraw Hill New York, 1977.

[5] R. Andonie and F. Petrescu., "Interacting systems and informational energy," *Foundation of Control Engineering*, no. 11, pp. 53–59, 1986.

[6] R. Andonie and A. Caţaron, "An informational energy LVQ approach for feature ranking," in *European Symposium on Artificial Neural Networks 2004, pages In d-side publications*, 2004, pp. 471–476.

[7] A. Caţaron and R. Andonie, "Energy generalized LVQ with relevance factors," in *Neural Networks, 2004. Proceedings. 2004 IEEE International Joint Conference on*, vol. 2, july 2004, pp. 1421 – 1426 vol.2.

[8] ——, "Informational energy kernel for LVQ," in *Proceedings of the 15th international conference on Artificial neural networks: formal models and their applications - Volume Part II*, ser. ICANN'05. Berlin, Heidelberg: Springer-Verlag, 2005, pp. 601–606.

[9] ——, "Energy supervised relevance neural gas for feature ranking," *Neural Processing Letters*, vol. 32, no. 1, pp. 59–73, 2010.

[10] ——, "How to infer the informational energy from small datasets," in *Proceedings of the 13th International Conference on Optimization of Electrical and Electronic Equipments: Optim 2012, May 24-26, 2012, Brasov, Romania*, 2012, pp. 1065–1070.

[11] A. Caţaron, R. Andonie, and Y. Chueh, "Asymptotically unbiased estimator of the informational energy with kNN," *International Journal of Computers, Communications and Control*, vol. 8, pp. 689–698, 2013.

[12] R. Hogg, *Introduction to mathematical statistics, 6/E*. Pearson Education, 2006.

[13] L. Faivishevsky and J. Goldberger, "ICA based on a smooth estimation of the differential entropy," in *NIPS*, 2008.

[14] C. Bishop, *Pattern recognition and machine learning*. New York: Springer, 2006.

[15] S. Nechifor, A. Petrescu, D. Damian, D. Puiu, and B. Tarnauca, "Predictive analytics based on CEP for logistic of sensitive goods," in *Proceedings of the 14th International Conference on Optimization of Electrical and Electronic Equipments: Optim 2014, May 22-24, 2014, Brasov, Romania*, 2014, pp. 817–822.