Amplifying Inter-message Distance: On Information Divergence Measures in Big Data

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Abstract

Message identification (M-I) divergence is an important measure of the information distance between probability distributions, similar to Kullback-Leibler (K-L) and Renyi divergence. In fact, M-I divergence with a variable parameter can make an effect on characterization of distinction between two distributions. Furthermore, by choosing an appropriate parameter of M-I divergence, it is possible to amplify the information distance between adjacent distributions while maintaining enough gap between two nonadjacent ones. Therefore, M-I divergence can play a vital role in distinguishing distributions more clearly. In this paper, we first define a parametric M-I divergence in the view of information theory and then present its major properties. In addition, we design a M-I divergence estimation algorithm by means of the ensemble estimator of the proposed weight kernel estimators, which can improve the convergence of mean squared error from $O(\Gamma^{-j/d})$ to $O(\Gamma^{-1})$ ($j \in (0, d]$). We also discuss the decision with M-I divergence for clustering or classification, and investigate its performance in a statistical sequence model of big data for the outlier detection problem.

Index Terms

Message Identification (M-I) Divergence, Discrete Distribution Estimation, Divergence Estimation, Big Data Analysis, Outlier Detection

I. INTRODUCTION

In the big data era, the amount of data from many kinds of areas is exploding greatly, and how to analyze the collected big data attracts more and more attention. For big data analysis, there are a series of relevant technologies including machine learning, pattern recognition, statistics, estimation

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theory and so on. As an essential element in machine learning, the information divergence can be used to deal with distribution problems by mapping the relationship between two probability distributions to nonnegative values. Currently, information divergences have been extended for nonnegative tensors and used to minimize the approximation error between the observed data and its model [1]. Additionally, typical applications of information divergences also include faulty detection [2], key frame selection [3], image and speech recognition [4], [?] and so on.

In the framework of the combination of information theory and big data analysis, information divergences were investigated as measures to handle the learning problem about distributions. In particular, the relative entropy as a special case of K-L divergence is a superior tool of measuring information distance in some applications such as anomaly detection [6], FMRI data processing [7], clustering and classification [8]. Moreover, Shannon entropy can be also regarded as a special case of K-L divergence with an uniform distribution. It is appropriate for entropy to be applied to intrinsic dimension estimation [9], texture classification and image registration [10]. In addition, information divergences can be applicable to extending methods of machine learning to distributional features [11].

Although there are a great deal of available information divergences, little research is investigated on how to select a better one for a certain application to big data. Due to the different properties of different divergences, this issue is a significant work for information divergences used in big data analysis. Besides, another factor which can contribute to the issue is that a divergence-based estimation may depend on the selected divergence in a given task. Then we can see that it is flexible for information divergences to cope with different data learning tasks. For example, Euclidean distance has superior performance on handling data with Gaussian noise; K-L divergence is suitable for topic collection of text documents [12]; Itakura-Saito divergence can perform well on audio signal processing [13]; as well as the MIM and non-parametric MIM which are similar to entropy, can be proven suitable for minority subset detection [14]–[16]. In addition, the information distance between given distributions can be also as a factor to make an effect on the divergence selection. Some divergences may not distinguish certain similar distributions due to the confusion between information distance and the statistical error.

In this paper, to study the information divergence as a measure in big data application, we will focus on the information distance measured by different divergences. As well, it is necessary to investigate the more efficient divergence estimation for practical applications or models. Before our work, let us review some typical information divergences first.
A. Information Divergence measures

There exist many different kinds of information divergences, which can play a vital role in the fields of information theory, statistics and big data analysis. To simply summarize a variety of information divergences, we focus on the most commonly used ones including K-L divergence, Renyi divergence and $\alpha$-, $\beta$- or $\gamma$-divergences [17]–[19], which belong to broader ones such as the f-divergences or Bregman divergences [20].

For two finite discrete distributions $P = (p_1, p_2, ..., p_n)$ and $Q = (q_1, q_2, ..., q_n)$, the definitions of the popularly used divergences and some of their special cases or relationships are given below.

a). K-L divergence is defined as

$$D(P \parallel Q) = \sum_i p_i \log \left( \frac{p_i}{q_i} \right).$$

(1)

b). Renyi divergence of order $\alpha$ is defined as

$$D_\alpha(P \parallel Q) = \frac{1}{\alpha - 1} \log \sum_i p_i^\alpha q_i^{1-\alpha},$$

(2)

where $0 < \alpha < \infty$, and $\alpha \neq 1$. Notes that in the case of $\alpha \to 1$, Renyi divergence converges to K-L divergence.

c). $\alpha$-divergence is defined as

$$D^{(\alpha)}(P \parallel Q) = \frac{\sum_i p_i^{\alpha} q_i^{1-\alpha} - \alpha p_i + (\alpha - 1) q_i}{\alpha(\alpha - 1)},$$

(3)

where $\alpha \to 1$, $\alpha = 2$, $\alpha = -1$ and $\alpha = 1/2$ denote K-L, Pearson Chi-square, inverse Pearson and double Hellinger distances, respectively.

d). $\beta$-divergence is defined as

$$D^{(\beta)}(P \parallel Q) = \frac{\sum_i p_i^{\beta+1} + \beta q_i^{(\beta+1)} - (\beta + 1) p_i q_i^{\beta}}{\beta(\beta + 1)},$$

(4)

where $\beta = 1$ and $\beta \to -1$ denote the Euclidean distance and Itakura-Saito divergence, respectively.

e). $\gamma$-divergence is defined as

$$D^{(\gamma)}(P \parallel Q) = \frac{1}{\gamma(\gamma + 1)} \left[ \log(\sum_i p_i^{\gamma + 1}) + \gamma \log(\sum_i q_i^{\gamma + 1}) - (\gamma + 1) \log(\sum_i p_i q_i^{\gamma}) \right],$$

(5)

where K-L divergence becomes its special case if $\gamma \to 0$.

However, there may be also situations where the commonly used divergences can not work well. To this end, we introduce a new divergence different from the above divergences as follows.
B. Message Identification Divergence

In this subsection, we shall introduce a new parametric information identification measure, which is referred to as the message identification divergence (M-I divergence).

**Definition 1.** For two given probability distributions with a same finite alphabet, \( P = (p_1, p_2, \ldots, p_n) \) and \( Q = (q_1, q_2, \ldots, q_n) \), the M-I divergence with parameter \( \varpi \) is defined as

\[
D_{MI}(P \parallel Q, \varpi) = D_{\varpi}(P \parallel Q) = \log \sum_{i=1}^{n} p_i e^{\left(\varpi \frac{p_i}{q_i}\right)} - \varpi,
\]

where \( \varpi > 0 \) is an adjustable identification parameter.

Note that the larger parameter \( \varpi \) is, the larger contribution the information distance elements \( p_i/q_i \) have to M-I divergence. In the application, it is necessary to set an appropriate \( \varpi \) which is not too large to compute easily.

C. Organization

The rest of this paper is organized as follows. In Section II, we discuss some major properties of M-I divergence, such as its monotonicity, convexity and inequality. In Section III, we propose a multidimensional kernel estimator with the weight window, which can be adapted to estimate a discrete distribution. As well, we discuss its performance in the mean squared error (MSE) criterion. Then an ensemble estimator for M-I divergence is also proposed by use of some weighted-window kernel estimators. Section IV discuss how to use M-I divergence in big data analysis and apply it to a proposed outlier detection model. Besides, some simulations are also presented to check our theoretical results. Finally, we conclude the paper in Section V.

II. THE PROPERTIES OF M-I DIVERGENCE

In this section, some dominant properties of M-I divergence is investigated in details.

A. The Non-negative Property

**Proposition 1.** The M-I divergence \( D_{\varpi}(P \parallel Q) \) with \( \varpi > 0 \) is non-negative for any probability \( P \) and \( Q \), namely

\[
D_{\varpi}(P \parallel Q) \geq 0.
\]

**Proof:** Define \( f(x) = \exp(\varpi x^{-1}) \) with \( \varpi > 0 \). It is readily seen that the second order derivative of \( f(x) \) with respect to \( x \) is positive, namely, \( \frac{\partial^2 f(x)}{\partial x^2} = \left(\varpi^2 x^{-4} + 2\varpi x^{-3}\right) e^{\varpi x^{-1}} > 0 \). Then, we know
that \( f(x) \) is a convex function for \( x \in \mathbb{R} \). According to Jensen’s inequality and the concavity of function \( \log(x) \), we have
\[
D_{\infty}(P \parallel Q) = \log \sum_{i=1}^{n} p_i e^{\frac{\log p_i}{q_i}} - \varpi \geq \log e^{\sum_{i=1}^{n} p_i \left( \frac{p_i}{q_i} \right)^{-1}} - \varpi = \log e^\varpi - \varpi = 0. \tag{8}
\]
In particular, the equality holds if and only if \( p_i = q_i \ (i \in \{1, 2, \ldots, n\}) \). 

**B. Monotonicity**

**Proposition 2.** For the identification parameter \( \varpi \in (0, +\infty) \), the M-I divergence \( D_{\infty}(P \parallel Q) \) is nondecreasing in \( \varpi \).

**Proof.** By using the definition of M-I divergence and dividing its support set of \( i \) into two parts, it is readily seen that the partial derivative of \( D_{\infty}(P||Q) \) with respect to \( \varpi \) satisfies
\[
\frac{\partial D_{\infty}(P \parallel Q)}{\partial \varpi} = \frac{\sum_{i \in \{i:p_i \geq q_i\} \cup \{i:p_i < q_i\}} \left( \frac{p_i}{q_i} - 1 \right) p_i e^{\frac{\varpi}{q_i}}}{\sum_i p_i e^{\frac{\varpi}{q_i}}} \geq \frac{\sum_{i \in \{i:p_i \geq q_i\}} \left( \frac{p_i}{q_i} - 1 \right) p_i e^{\varpi} + \sum_{i \in \{i:p_i < q_i\}} \left( \frac{p_i}{q_i} - 1 \right) p_i e^{\varpi}}{\sum_i p_i e^{\frac{\varpi}{q_i}}} = \frac{e^{\varpi} \sum_i \left( \frac{p_i}{q_i} - 1 \right) p_i}{\sum_i p_i e^{\frac{\varpi}{q_i}}}. \tag{9}
\]
According to Jensen’s inequality, it is readily seen that \( e^{\varpi} \sum_i \left( \frac{p_i}{q_i} - 1 \right) p_i \geq e^{\varpi} \left[ \left( \sum_i p_i \frac{q_i}{p_i} \right)^{-1} - 1 \right] \). Thus, it can be readily verified that
\[
\frac{\partial D_{\infty}(P \parallel Q)}{\partial \varpi} \geq \frac{e^{\varpi} \left[ \left( \sum_i p_i \frac{q_i}{p_i} \right)^{-1} - 1 \right]}{\sum_i p_i e^{\frac{\varpi}{q_i}}} = 0, \tag{10}
\]
which means \( D_{\infty}(P \parallel Q) \) is monotonically nondecreasing in \( \varpi \) and the property is proved.

**Remark 1.** If and only if \( p_i = q_i \ (i \in \{1, 2, \ldots, n\}) \), M-I divergence \( D_{\infty}(P \parallel Q) \) remains zero with increasing \( \varpi \). In other cases \( (p_i \neq q_i) \), \( D_{\infty}(P \parallel Q) \) is increasing in \( \varpi \). According to this property, it can be apparently deduced that \( \varpi \) is an adjustable parameter for M-I divergence to amplify the distance between different probability distributions.

**C. The Convexity Property**

**Proposition 3.** For any \( \varpi > 0 \), M-I divergence \( D_{\infty}(P \parallel Q) \) is jointly convex in the case of exponential function. That is, for two given pairs of probability distributions \( (P_0, Q_0) \) and \( (P_1, Q_1) \) without zero elements, and any \( 0 < \lambda < 1 \), we have
\[
(1 - \lambda) e^{D_{\infty}(P_0\parallel Q_0)} + \lambda e^{D_{\infty}(P_1\parallel Q_1)} \geq e^{D_{\infty}(P_\lambda\parallel Q_\lambda)}, \tag{11}
\]
where \( P_\lambda = (1 - \lambda)P_0 + \lambda P_1 \) and \( Q_\lambda = (1 - \lambda)Q_0 + \lambda Q_1 \).

**Proof.** Define \( f(x) = xe^{\varpi x} \) with \( \varpi > 0 \) and \( x \in \mathbb{R} \). It is easy to see that the first order and the second order derivative of \( f(x) \) are both positive for \( \varpi > 0 \) and \( x > 0 \). Then, it is evident that \( f(x) \) is convex for \( \varpi > 0 \) and \( x > 0 \). By using Jensen’s inequality, in the case of \( \varpi > 0 \), we have

\[
(1 - \lambda)\frac{q_{0,i}}{q_{\lambda,i}} \left( \frac{p_{0,i}}{q_{0,i}} \right) e^{\varpi \left( \frac{p_{0,i}}{q_{0,i}} \right)} + \lambda \frac{q_{1,i}}{q_{\lambda,i}} \left( \frac{p_{1,i}}{q_{1,i}} \right) e^{\varpi \left( \frac{p_{1,i}}{q_{1,i}} \right)} \\
\geq \left( \frac{p_{\lambda,i}}{q_{\lambda,i}} \right) e^{\varpi \left( \frac{p_{\lambda,i}}{q_{\lambda,i}} \right)},
\]

(12)

where \( p_{\lambda,i} = (1 - \lambda)p_{0,i} + \lambda p_{1,i} \) and \( q_{\lambda,i} = (1 - \lambda)q_{0,i} + \lambda q_{1,i} \), as well as, \( p_{m,i} \) and \( q_{m,i} \) \((m = 0, 1, \lambda; \ i = 0, 1, ..., n)\) are any elements in \( P_m \) and \( Q_m \) \((m = 0, 1, \lambda)\), respectively.

Then, for all elements of probability distributions \( P_m \) and \( Q_m \) \((m = 0, 1, \lambda)\), we have

\[
(1 - \lambda) \sum_i p_{0,i} e^{\varpi \left( \frac{p_{0,i}}{q_{0,i}} \right)} + \lambda \sum_i p_{1,i} e^{\varpi \left( \frac{p_{1,i}}{q_{1,i}} \right)} \geq \sum_i p_{\lambda,i} e^{\varpi \left( \frac{p_{\lambda,i}}{q_{\lambda,i}} \right)}
\]

(13)

for any \( \varpi > 0 \), which proves the property.

**Corollary 1.** For any two pairs of probability distributions \((P_0, Q_0)\) and \((P_1, Q_1)\) without zero elements, and any \( \lambda \in (0, 1) \), we have

\[
\max\{D_\varpi(P_0 \parallel Q_0), D_\varpi(P_1 \parallel Q_1)\} \geq D_\varpi(P_\lambda \parallel Q_\lambda),
\]

(14)

where \( P_\lambda = (1 - \lambda)P_0 + \lambda P_1 \) and \( Q_\lambda = (1 - \lambda)Q_0 + \lambda Q_1 \).

**Proof.**. In view of the convexity property of M-I divergence \( D_\varpi(P \parallel Q) \), in the case of exponential function, we have

\[
(1 - \lambda) \max\{e^{D_\varpi(P_0 \parallel Q_0)}, e^{D_\varpi(P_1 \parallel Q_1)}\} + \lambda \max\{e^{D_\varpi(P_0 \parallel Q_0)}, e^{D_\varpi(P_1 \parallel Q_1)}\} \geq e^{D_\varpi(P_\lambda \parallel Q_\lambda)}.
\]

(15)

As a result, it can be easily seen that

\[
\max\{e^{D_\varpi(P_0 \parallel Q_0)}, e^{D_\varpi(P_1 \parallel Q_1)}\} \geq e^{D_\varpi(P_\lambda \parallel Q_\lambda)}.
\]

(16)

Further, we can gain this corollary by use of the monotonicity of exponential function.

**Corollary 2.** For any probability distributions \( P, Q_0 \) and \( Q_1 \) which consist of positive elements, and \( \lambda \in (0, 1) \), we have,

\[
(1 - \lambda) e^{D_\varpi(P \parallel Q_0)} + \lambda e^{D_\varpi(P \parallel Q_1)} \geq e^{D_\varpi(P \parallel (1 - \lambda)Q_0 + \lambda Q_1)}.
\]

(17)

This can be verified by substituting \( p \) for \( p_0 \) and \( p_1 \) in the convexity property.
D. The Inequality Property

Proposition 4. For two given probability distributions with the finite support set, \( P = (p_1, p_2, ..., p_n) \) and \( Q = (q_1, q_2, ..., q_n) \) (\( p_i > 0, q_i > 0, i = 1, 2, ..., n \)), the relationship among M-I divergence \( D_\varpi(P \parallel Q) \), K-L divergence \( D(P \parallel Q) \) and Renyi divergence \( D_\alpha(P \parallel Q) \) can be indicated as

\[
D_\varpi(P \parallel Q) \geq D(P \parallel Q) \geq D_\alpha(P \parallel Q), \tag{18}
\]

where \( \varpi \geq 1 \) and \( \alpha \in [0, 1] \).

Proof: Define a function \( f(x) = e^{\varpi(x-1)} - x \) with \( \varpi > 0 \) and \( x \in (0, +\infty) \). By setting \( \frac{\partial f(x)}{\partial x} = 0 \), it can be readily testified that the minimum of \( f(x) \) is obtained at \( x_0 = 1 + \frac{1}{\varpi} \log \frac{1}{\varpi} \). Furthermore, it is not difficult to see that only when \( \varpi = 1 \), can \( f(x_0, \varpi = 1) = 0 \). Therefore, it is clear to see that

\[
f(x) = e^{\varpi(x-1)} - x \geq 0, \tag{19}
\]

where \( \varpi = 1, x \in (0, +\infty) \) and \( f(x) = 0 \) for \( x = 1 \).

Now, the proof of left hand side inequality in Eq. (18) can be cast into the proof of \( D_\varpi(P \parallel Q) \geq D(P \parallel Q) \) with \( \varpi = 1 \). This is due to the monotonicity of \( D_\varpi(P \parallel Q) \) in Proposition 2.

By averaging \( f(\frac{p_i}{q_i}) \) in the distribution \( P = (p_1, p_2, ..., p_n) \) and considering the concavity of logarithmic function, we have \( \log \sum_i p_i e^{\varpi(\frac{p_i}{q_i} - 1)} - \log \sum_i p_i \frac{p_i}{q_i} \geq 0 \), with \( \varpi = 1 \). As well, in virtue of Jensen’s inequality, it is apparent that

\[
\log \sum_i p_i e^{\varpi(\frac{p_i}{q_i} - 1)} - \sum_i p_i \log \frac{p_i}{q_i} \geq 0, \tag{20}
\]

which implies that \( D_\varpi(P \parallel Q) \geq D(P \parallel Q) \) does work for \( \varpi \geq 1 \) due to the monotonicity of M-I divergence.

Furthermore, \( D_\alpha(P \parallel Q) \) keeps increasing in the order of \( \alpha \), mentioned in Theorem 3 of [21]. Correspondingly, we have

\[
D(P \parallel Q) = \sup_{0<\alpha<1} D_\alpha(P \parallel Q). \tag{21}
\]

Therefore, by combining Eq. (20) and Eq. (21), the inequality property of \( D_\varpi(P \parallel Q) \) can be proved readily.

Remark 2. According to the inequality property, the distance between two adjacent distributions can be amplified by the measure of M-I divergence. Moreover, M-I divergence is more sensitive than the other divergences to measure the distance between two nonadjacent distributions. Thus, it is more efficient for M-I divergence to distinguish two distributions.
III. Estimation of M-I Divergence

A. The Multidimensional Discrete Kernel Estimator

1) Multidimensional Kernel with Weight Window:

With regard to the discrete kernel, there is a general definition to characterize it specifically according to [22] as follows.

**Definition 2.** Let \( S \) be the finite support of the unknown probability mass function (p.m.f), to be estimated, with \( x_i \) an element in \( S \). A p.m.f \( K_{x_i,s}(\cdot) \) on support \( S \) (not depending on \( s \)) is regarded as a discrete kernel with the parameter \( s > 0 \), if it satisfies the following conditions:

\[
\begin{align*}
  x_i &\in S, \quad (22a) \\
  \lim_{s \to 0} \mathbb{E}(Z_{x_i,s}) &= x_i, \quad (22b) \\
  \lim_{s \to 0} \text{Var}(Z_{x_i,s}) &= 0, \quad (22c)
\end{align*}
\]

where \( Z_{x_i,s} \) is a discrete random variable with p.m.f \( K_{x_i,s}(\cdot) \).

Based on the above characteristics of the discrete kernel, some special kernel functions can be designed in various ways. As well, we present a kernel estimator with the weight window for multidimensional discrete distribution as follows.

**Definition 3.** Let \( X_1, X_2, ..., X_N \) be independent and identically distributed (i.i.d) multidimensional random variables with \( d \)-dimensional multivariate p.m.f \( p(x_i) \) on finite support \( U = [a_1, a_2, ..., a_L]^d \). A discrete kernel estimator \( \tilde{p}_s(x_i) \) with a weight window is defined as

\[
\tilde{p}_s(x_i) = \frac{1}{N} \sum_{k=1}^{N} K_{x_i,s,d} (X_k) = \frac{1}{N} \sum_{k=1}^{N} \sum_{x \in U} W(s, x_i, x_j) I_{\{X_k = x_j\}}, \quad x_i, j \in U,
\]

in which the weight window function is

\[
W(s, x_i, x_j) = \begin{cases} 
1 - s, & |x_i^u - x_j^u| = 0 \\
\frac{s}{(2 \tilde{d} + 1)^d - 1}, & 0 < |x_i^u - x_j^u| \leq \tilde{d} \\
0, & |x_i^u - x_j^u| > \tilde{d}
\end{cases}
\]

where \( u \in \{1, 2, ..., d\} \) denotes the dimension order, \( s \) is a smoothing parameter, the window size \( \tilde{d} \) is the distance of support indexes between \( x_i \) and \( x_j \) in every dimension, \( L \) is the size of support indexes in every dimension, \( I_{\{X_k = x_j\}} \) is the indicator function and \( K_{x_i,s,d} \) is the kernel function with \( 0 \leq s < 1, \ x_i \in U \) and \( \tilde{d} < \frac{L-1}{2} \).
From the above definition of multidimensional kernel estimator with the weight window, it can be clearly noted that when the smoothing parameter (or weight parameter) satisfies $s = 0$, the discrete weight window function $W(s, x_i, x_j)$ degenerates into the indicator function $I_{\{x_i = x_j\}}$. As well, it is readily seen that regardless of weight parameter $s$ or variable $x_i$, the sum of $W(s, x_i, x_j)$ for all $x_j \in \{x_j : 0 \leq |x_i^n - x_j^m| \leq \tilde{d}, x_j \in U\}$ fulfills
\[
\sum_{x_j \in U} W(s, x_i, x_j) = 1.
\] (25)

**Remark 3.** As far as the kernel estimator $\tilde{p}_s(x_i)$ is concerned, it is the core idea that relative frequencies derived from plug-in estimator are weighted to constitute the p.m.f estimator. In this way, more information of samples can be made use of to estimate every probability element in p.m.f. Furthermore, it is implied that the performance of the estimator $\tilde{p}_s(x_i)$ mainly depends on the selection of weight parameter in the case of the given p.m.f and known samples. In addition, if the weight parameter $s$ tends to zero as $N \to +\infty$, the estimator $\tilde{p}_s(x_i)$ will tend to the real $p(x_i)$.

2) Selection of Kernel Weight Parameter:

We now consider selecting the weight parameter $s$, which can make an effect on the performance of kernel estimator. In general, the mean squared error (MSE) is accepted as a performance criterion for estimators. For a given $d$-dimensional multivariate p.m.f $p(x_i)$ and its kernel estimator $\tilde{p}_s(x_i)$, the MSE can be treated as a function of $s$ as follows,
\[
f_{\text{MSE}}(s) = \mathbb{E} \sum_{x_i \in U} [\tilde{p}_s(x_i) - p(x_i)]^2
= \sum_{x_i \in U} \text{Var} [\tilde{p}_s(x_i)] + \sum_{x_i \in U} \text{Bias}^2 [\tilde{p}_s(x_i)]
= \frac{1}{N} \sum_{x_i \in U} \sum_{x_j \in U} W^2(s, x_i, x_j)p(x_j) - \frac{1}{N} \sum_{x_i \in U} \left[ \sum_{x_j \in U} W(s, x_i, x_j)p(x_j) \right]^2
+ \sum_{x_i \in U} \left[ \sum_{x_j \in U} W(s, x_i, x_j)p(x_j) - p(x_i) \right]^2.
\] (26)

What is more, it is readily realized that a value of $s$ can be provided by minimizing the MSE with respect to $s$. In that case, the optimal weight parameter is given by
\[
s_0 = \arg \min_{0 \leq s < 1} f_{\text{MSE}}(s).
\] (27)
By substituting Eq. (24) into Eq. (26), we have

\[
f_{\text{MSE}}(s) = \frac{1 - \sum_{x_i \in U} p^2(x_i)}{N} + \frac{2}{N} \sum_{x_i \in U} \left\{ p^2(x_i) - p(x_i) \frac{N p(x_i) \sum_{x_j \in V_d} p(x_j)}{(2d + 1)^d - 1} \right\} \tag{28}
\]

\[
+ \frac{1}{N} \sum_{x_i \in U} \left\{ (N - 1)p^2(x_i) + p(x_i) + \frac{\sum_{x_j \in V_d} p(x_j) + (N - 1) \left[ \sum_{x_j \in V_d} p(x_j) \right]^2}{(2d + 1)^d - 1} \right\} \quad \text{s}^2,
\]

where the set \( V_d \) denotes \( \{ \tilde{x}_j : 0 < |\tilde{x}_j^u - x_i^u| \leq \tilde{d}, \tilde{x}_j \in U \} \).

By setting \( \frac{\partial f_{\text{MSE}}(s)}{\partial s} = 0 \), we can gain the minimum value of \( f_{\text{MSE}}(s) \). Therefore, it is readily seen that the optimal weight parameter is

\[
s_0 = \frac{1 - \sum_{x_i \in U} p^2(x_i) + \frac{\sum_{x_i \in U} \sum_{x_j \in V_d} p(x_i) p(x_j)}{(2d + 1)^d - 1}}{\Phi(p, N, \tilde{d})}, \tag{29}
\]

where the denominator is a function of \( p \), \( N \), and \( \tilde{d} \), as

\[
\Phi(p, N, \tilde{d}) = 1 + \frac{\sum_{x_i \in U} \sum_{x_j \in V_d} p(x_j)}{(2\tilde{d} + 1)^d - 1} + (N - 1) \left\{ \sum_{x_i \in U} p^2(x_i) + \frac{\sum_{x_i \in U} \left[ \sum_{x_j \in V_d} p(x_j) \right]^2}{(2\tilde{d} + 1)^d - 1} - \frac{2 \sum_{x_i \in U} \sum_{x_j \in V_d} p(x_i) p(x_j)}{(2\tilde{d} + 1)^d - 1} \right\}. \tag{30}
\]

It is worth noting that the optimal weight parameter \( s_0 \) depends on the p.m.f \( p(x_i) \), the number of multidimensional random variables \( N \) and the distance \( \tilde{d} \). However, the p.m.f is hardly known and needs estimating. For this reason, it can be thought over to replace the unknown \( p(x_i) \) with a consistent estimator, plug-in estimator \( \hat{p}(x_i) \). In that case, the suboptimal but practical solution \( \hat{s}_0 \) of weight parameter under the MSE criterion is put forward as

\[
\hat{s}_0 = \frac{1 - \sum_{x_i \in U} \hat{p}^2(x_i) + \frac{\sum_{x_i \in U} \sum_{x_j \in V_d} \hat{p}(x_i) \hat{p}(x_j)}{(2d + 1)^d - 1}}{\Phi(\hat{p}, N, \tilde{d})}. \tag{31}
\]

**Remark 4.** For a given p.m.f \( p(x_i) \) and \( \tilde{d} \), it is readily seen that the suboptimal weight parameter satisfies \( \hat{s}_0 = O(1/N) \), which is similar to the optimal \( s_0 \). Moreover, if the weight parameter \( s \) is replaced by \( \hat{s}_0 \), \( f_{\text{MSE}}(\hat{s}_0) \) will tend to zero as \( N \to +\infty \). That is, the estimator \( \bar{p}_{\hat{s}_0}(x_i) \) tends to the real \( p(x_i) \) in the MSE criterion.
3) Performance Analysis:

In the view of MSE criterion, the multidimensional window kernel estimator \( \hat{\psi}_{\bar{s}_0}(x_i) \) keeps the same large-sample properties as plug-in estimator \( \hat{p}(x_i) \). However, it arises a question whether the former is superior to the latter in the performance of estimation. In order to distinguish which one is better, the measurements of MSE with respect to \( \bar{s}_0(x_i) \) and \( \hat{p}(x_i) \) are given respectively by

\[
\text{MSE}(\bar{s}_0) = f_{\text{MSE}}(\bar{s}_0),
\]

\[
\text{MSE}(\hat{p}) = E \sum_{x_i \in U} \left( \hat{p}(x_i) - p(x_i) \right)^2.
\]

Considering the definition of plug-in estimator, \( \hat{p}(x_i) = \frac{1}{N} \sum_{k=1}^{N} I(x_k = x_i) \), we have

\[
\text{MSE}(\hat{p}) = \sum_{x_i \in U} \left\{ E \left[ \hat{p}^2(x_i) \right] - p^2(x_i) \right\}
\]

\[
= \sum_{x_i \in U} \left[ \frac{p(x_i) + (N - 1)p^2(x_i)}{N} - p^2(x_i) \right]
\]

\[
= 1 - \frac{\sum_{x_i \in U} p^2(x_i)}{N}.
\]

By replacing \( \bar{s} \) with \( \bar{s}_0 \) in Eq. (28), the difference of the two MSE functions can be written as

\[
\text{MSE}(\hat{p}) - \text{MSE}(\hat{p}) = \phi(\hat{p}, N, \tilde{d})\bar{s}_0 + \psi(\hat{p}, N, \tilde{d})\bar{s}_0^2,
\]

where \( \phi(\hat{p}, N, \tilde{d}) \) and \( \psi(\hat{p}, N, \tilde{d}) \) are both functions of \( p \), \( N \) and \( \tilde{d} \). What is more, it is apparent that the convergence of \( \phi(\hat{p}, N, \tilde{d}) \) and \( \psi(\hat{p}, N, \tilde{d}) \) are \( O(1) + O(1/N) \).

Due to the fact that the parameter \( \bar{s}_0 \to 0 \) as \( N \to +\infty \), the \( \psi(\hat{p}, N, \tilde{d})\bar{s}_0^2 = O(\bar{s}_0^2) \) tends to zero at a faster rate than \( \phi(\hat{p}, N, \tilde{d})\bar{s}_0 \), as \( N \) increasing. That is, the first term \( \phi(\hat{p}, N, \tilde{d})\bar{s}_0 \) dominates the positive or negative nature of Eq. (34). In addition, it is not difficult to know that \( \phi(\hat{p}, N, \tilde{d}) < 0 \) always holds by virtue of \( p^2(x_i) - p(x_i) \leq 0 \) in the second term of Eq. (28). Therefore, it is sure that for large enough \( N \), \( \text{MSE}(\hat{p}) < \text{MSE}(\hat{p}) \) holds for any p.m.f \( p(x_i) \neq 0 \). This implies that \( \bar{s}_0(x_i) \) has better performance than \( \hat{p}(x_i) \) in the MSE criterion.

B. Multidimensional Weighted Ensemble Estimation

For an ensemble of estimators \{ \hat{D}_{l_1}, \hat{D}_{l_2}, ..., \hat{D}_{l_T} \} of a parameter \( D \), the weighted ensemble estimator with respect to the weight \( \lambda = \{ \lambda_{l_1}, \lambda_{l_2}, ..., \lambda_{l_T} \} \) is defined as

\[
\hat{D}_\lambda = \sum_{l \in \bar{I}} \lambda_l \hat{D}_l,
\]

where the \( \bar{I} = \{ l_1, l_2, ..., l_T \} \) denotes an index set. As well, the ensemble of weights is constrained by \( \sum_{l \in \bar{I}} \lambda_l = 1 \), which can ensure that the weighted ensemble estimator \( \hat{D}_\lambda \) holds asymptotically unbiased in the case of the asymptotically unbiased estimators \{ \hat{D}_{l_1}, \hat{D}_{l_2}, ..., \hat{D}_{l_T} \}.
Theorem 1. Assume the bias and variance of every estimator $\hat{D}_l$ ($l \in \bar{l}$) satisfy the following conditions, respectively:

$$\text{Bias}(\hat{D}_l) = \sum_{j \in J} \gamma_j \varphi_j(l) \Gamma^{-j/2d} + \rho_{\text{bias}}(\Gamma^{-1/2}), \quad (36a)$$

$$\text{Var}(\hat{D}_l) = \rho_{\text{var}}(\Gamma^{-1/2}), \quad (36b)$$

where $\gamma_j$ are constants depending on a $d$-dimensional p.m.f $p(x_i)$, $d$ is the dimension number, $J = \{j_i : 0 < j_i \leq d, 1 \leq i \leq I \}$ denotes an index set, $\Gamma$ is the number of samples, $\varphi_j(l)$ are independent functions of index $l$, and $\rho_{\tau}(\Gamma^{-1/2})$ with any subscript $\tau$ are functions of $\Gamma^{-1/2}$. Then, there exists a weight vector $\mathbf{X}^*$ leading to

$$\text{MSE}(\hat{D}_{\mathbf{X}^*}) = \mathbb{E} \left[ (\hat{D}_{\mathbf{X}^*} - D)^2 \right] \leq \rho_{\mathbf{X}^*}(\Gamma^{-1/2}). \quad (37)$$

The weight vector $\mathbf{X}^*$ is given by solving the following optimization problem:

$$\mathbf{X}^* = \arg \min_{\mathbf{X}} \|\mathbf{X}\|^2$$

subject to:

$$\begin{align*}
\sum_{l \in \bar{l}} \lambda_l &= 1, \\
\sum_{l \in \bar{l}} \lambda_l \varphi_j(l) &= 0, j \in J.
\end{align*} \quad (38)$$

Proof: For the ensemble of estimators $\{\hat{D}_l\}_{l \in \bar{l}}$, the bias of the weighted ensemble estimator $\hat{D}_\mathbf{X}$ is given by

$$\text{Bias}(\hat{D}_\mathbf{X}) = \mathbb{E} \left\{ \sum_{l \in \bar{l}} \lambda_l \hat{D}_l - D \right\} = \sum_{l \in \bar{l}} \lambda_l \text{Bias}(\hat{D}_l)$$

$$= \sum_{l \in \bar{l}} \sum_{j \in J} \gamma_j \lambda_l \varphi_j(l) \Gamma^{-j/2d} + \rho_{\lambda_{\text{bias}}}(\Gamma^{-1/2}). \quad (39)$$

Considering the Cauchy-Schwartz inequality, it is not difficult to derive the variance of $\hat{D}_\mathbf{X}$ as follows:

$$\text{Var}(\hat{D}_\mathbf{X}) = \mathbb{E} \left\{ \sum_{l \in \bar{l}} \lambda_l [\hat{D}_l - \mathbb{E}(\hat{D}_l)] \right\}^2 \leq \sum_{l \in \bar{l}} \lambda_l^2 \sum_{l \in \bar{l}} \mathbb{E} \left[ \hat{D}_l - \mathbb{E}(\hat{D}_l) \right]^2 = \|\mathbf{X}\|^2 \text{Var}(\hat{D}_l). \quad (40)$$

According to the condition $I \leq T - 1$, it is readily seen that there exists at least one solution for the constraint conditions of Eq. (38). Thus, there is a solution to minimize $\|\mathbf{X}\|^2$, which can reduce the bias of the ensemble estimator to $\rho_{\lambda_{\text{bias}}}(\Gamma^{-1/2})$ and limit the contribution of the variance. Then, the MSE of ensemble estimator with respect to the optimal solution $\mathbf{X}^*$ can be derived as

$$\text{MSE}(\hat{D}_{\mathbf{X}^*}) = \text{Bias}^2(\hat{D}_{\mathbf{X}^*}) + \text{Var}(\hat{D}_{\mathbf{X}^*})$$

$$\leq \rho_{\mathbf{X}^*_{\text{bias}}}(\Gamma^{-1/2}) + \|\mathbf{X}^*\|^2 \rho_{\mathbf{X}^*_{\text{var}}}(\Gamma^{-1/2}) \leq \rho_{\mathbf{X}^*}(\Gamma^{-1/2}), \quad (41)$$
which can verify the theorem.

In addition, from Theorem 1, it is not difficult to derive the corollary 3 by replacing functions $\rho_{\tau}(\cdot)$ with order $O(\cdot)$ or $o(\cdot)$ as follows.

**Corollary 3.** For the bias and variance of the ensemble of estimators $\{\hat{D}_l\}_{l \in \mathbb{I}}$, the following conditions are satisfied as

$$
\text{Bias}(\hat{D}_l) = \sum_{j \in J} \gamma_j \varphi_j(l) \Gamma^{-j/2d} + o\left( \Gamma^{-1/2} \right), 
$$

$$
\text{Var}(\hat{D}_l) = O\left( \Gamma^{-1} \right).
$$

Then, there exists a weight vector $\lambda^*$ given by Eq. (38), which can lead to

$$
\text{MSE}(\hat{D}_{\lambda^*}) = O\left( \Gamma^{-1} \right).
$$

In order to obtain the above convergence rate of MSE, it is sufficient for $\sum_{l \in \mathbb{I}} \lambda_l \varphi_j(l) \Gamma^{-j/2d}$ to be of order $O(\Gamma^{-1/2})$. Thus, the optimal weight vector can be determined as

$$
\lambda^* = \arg \min_{\lambda} \delta \\
\text{s.t. } \sum_{l \in \mathbb{I}} \lambda_l = 1, \\
\left| \sum_{l \in \mathbb{I}} \lambda_l \varphi_j(l) \Gamma^{1/2-j/2d} \right| \leq \delta, \quad j \in J, \\
||\lambda||_2^2 \leq \epsilon,
$$

where the parameter $\epsilon$ is small enough.

**Remark 5.** For the weighted ensemble estimator, on the one hand, it possesses a distinctive superiority that the MSE is endowed with faster convergence by using the weight vector to eliminate the higher order bias terms. On the other hand, it is visible that the weighted estimator applies to the circumstance where there are estimators with different indexes.

C. Ensemble Estimator for M-I Divergence

In this subsection, we focus on the estimation of M-I divergence between two $d$-dimensional multivariate distributions $P$ and $Q$ whose p.m.f.s are $p(x_i)$ and $q(x_i)$ with the known finite support $\mathbb{U} = [a_1, a_2, ..., a_L]^d$. In terms of the definition of M-I divergence, it is apparent that the estimator of M-I divergence depends on the estimator of $F_{\omega}(P \parallel Q) = \sum_{x_i \in \mathbb{U}} p(x_i) e^{\frac{\pi_{x_i}^p}{\pi_{x_i}^q}}$, which can be approximately calculated by using the samples splitting approach as follows.
Assume that the i.i.d. random samples from $P$ are divided into two parts $\{X_1, \ldots, X_N\}$ and $\{X_{N+1}, \ldots, X_{N+M}\}$. The latter part is used to estimate the p.m.f of $P$ at the $N$ points $\{X_1, \ldots, X_N\}$ by means of the weighted-window kernel. Similarly, the weighted-window kernel estimator of the p.m.f of $Q$ at the $N$ points $\{X_1, \ldots, X_N\}$ is calculated by use of the i.i.d. samples $\{Y_1, \ldots, Y_M\}$ drawn from $Q$. Then the estimator of $F_\varpi(P \parallel Q)$ can be written as
\[
\hat{F}_d = \frac{1}{N} \sum_{i=1}^{N} e^{\varpi \tilde{p}_{\hat{s}_0}(X_i) \tilde{q}_{\hat{s}_0}(X_i)},
\] (45)
where $\tilde{p}_{\hat{s}_0}$ and $\tilde{q}_{\hat{s}_0}$ are weighted-window kernel estimators with the distance $\tilde{d}$ mentioned in the subsection III-A.

**Theorem 2.** The bias of the estimator $\hat{F}_d$ with weighted-window kernel is given by
\[
\text{Bias}(\hat{F}_d) = \sum_{j \in J} b_j \left( \frac{K}{M} \right)^{j/d} + o\left( \frac{K}{M} \right) + o\left( \frac{1}{K} \right) + O\left( \frac{1}{M} \right),
\] (46)
where $K = \left[ \frac{(2\tilde{d}+1)}{L} \right]^d M$ is a real number determined by $\tilde{d} < \frac{L-1}{2}$ and the parameter $b_j$ are constants depending on the distributions $P$ and $Q$.

**Theorem 3.** The variance of the estimator $\hat{F}_d$ with weighted-window kernel is given by
\[
\text{Var}(\hat{F}_d) = O\left( \frac{1}{N} \right).
\] (47)

The proof of Theorem 2 and 3 are given in Appendix A and B.

For a positive $T \geq I + 1$ and a positive real number set $\tilde{l} = \{l_1, \ldots, l_T\}$, let $K = \Delta \sqrt{M}$, $\Delta = \left[ \frac{(2\tilde{d}+1)}{L} \right]^d \sqrt{M}$, $l \in \tilde{l}$, $M = \mu \Gamma$ and $N = (1 - \mu) \Gamma$ with $0 < \mu < 1$. Note that the $l$ indexes over the distance size $\tilde{d}$ for the weighted-window kernel estimator. Then, the ensemble estimator of $\hat{F}_d$ is given by
\[
\hat{F}_\lambda = \sum_{l \in \tilde{l}} \lambda_l \hat{F}_{d_l},
\] (48)
where $\hat{F}_{d_l}$ denotes a $\hat{F}_d$ with an index $l$ for different $\tilde{d}$.

From Theorem 2 and 3, it is readily seen that the biases and variances of the ensemble estimators satisfy the conditions mentioned in Eq. (42a) when $\varphi_j(l) = \Delta^{j/d}$ and $J = \{1, \ldots, d\}$. Therefore, it is available to find the optimal $\lambda^*$ by using Corollary 3 so that we can improve the MSE convergence for the estimation of $F_\varpi(P \parallel Q)$. That is, we can make good use of the better estimator $\hat{F}_\lambda^*$ to obtain the better estimator of M-I divergence as
\[
\hat{D}_\varpi(P \parallel Q) = \log \hat{F}_\lambda^* - \varpi.
\] (49)
In addition, it is easily to see that the MSE of $\hat{D}_\varpi(P \parallel Q)$ is given by
\[
\text{MSE}(\hat{D}_\varpi(P \parallel Q)) = O(\Gamma^{-1}),
\] (50)
whose proof is given in Appendix C.

In order to summarize the above process more specifically, the ensemble estimator with weighted-window kernel for M-I divergence is listed in Algorithm 1.

**Algorithm 1** Optimally weighted ensemble estimator with window kernel for M-I divergence

**Input:** $\mu, \varepsilon, L$, the distance set $\{d_l : l \in \overline{l}\}$ with the index set $\overline{l}$, samples set $\{Y_1, ..., Y_M\}$ from distribution $Q$, samples set $\{X_1, ..., X_M\}$ from distribution $P$, dimension $d$, the parameter $\varpi$ of M-I divergence.

**Output:** The optimally weighted ensemble estimator $\hat{D}_\varpi$.

1: $M \leftarrow \mu \Gamma$, $N \leftarrow \Gamma - M$
2: calculate the $\lambda^*$ by use of Eq. (44) with $\varphi_j(l) = \Delta^{j/d}$, $\Delta = \left[\frac{2d_l+1}{L}\right]^d \sqrt{M}$, $j \in \{1, ..., d\}$ and $l \in \overline{l}$.
3: for all $l \in \overline{l}$ do
4: $\tilde{d}_l \leftarrow$ choosing a distance by $l \in \overline{l}$
5: for all $X_i \in \{X_1, ..., X_N\}$ do
6: $\hat{p}(X_i)$ and $\hat{q}(X_i) \leftarrow \frac{1}{M} \sum_{k=N+1}^{N+M} I_{\{X_k = X_i\}}$ and $\frac{1}{M} \sum_{k=1}^{M} I_{\{Y_k = X_i\}}$, respectively.
7: smoothing parameters $\hat{s}_0(p)$ and $\hat{s}_0(q) \leftarrow$ using Eq. (31) with $M$, $\tilde{d}_l$, $\hat{p}(X_i)$ and $\hat{q}(X_i)$.
8: $\tilde{p}_0(p)(X_i)$ and $\tilde{q}_0(q)(X_i) \leftarrow$ make full use of $\hat{s}_0(p)$, $\hat{s}_0(q)$, $\hat{p}(X_i)$ and $\hat{q}(X_i)$ to calculate the two weighted-window kernel estimators by adopting Eq. (23) in definition 3.
9: end for
10: $\tilde{F}_{\lambda_l} \leftarrow \frac{1}{N} \sum_{i=1}^{N} e^{\tilde{p}_0(p)(X_i) \tilde{q}_0(q)(X_i)}$
11: end for
12: $\tilde{F}_{\lambda} \leftarrow \sum_{l \in \overline{l}} \lambda^*_l \tilde{F}_{\lambda_l}$
13: $\hat{D}_\varpi \leftarrow \log \tilde{F}_{\lambda} - \varpi$

**IV. APPLICATION TO BIG DATA ANALYSIS**

In this section, we will discuss how to exploit divergence measures to classify or cluster the data belonging to different distributions. In particular, we take into account the following detection problem about outlier or minority sequences in a set of sequences.

**A. The Model with Unknown Number of Outliers**

Assume that among a number of sample sequences, there are an unknown number of outlier sequences to be detected. The i.i.d. samples in the typical sequences are gained from a known distribution $P_t$, while
in the outlier sequences, the i.i.d. samples are taken from an unknown distribution \( Q_f \). In order to design a test to detect the outlier sequences, it is necessary to construct a model applying to the problem.

Consider \( T_0 \) independent sequences (\( T_0 \geq 3 \)), each of which can be denoted by \( \mathcal{X}^{(i)} \) for \( i = 1, \ldots, T_0 \). As well, each \( \mathcal{X}^{(i)} \) consists of \( I_0 \) i.i.d samples \( \{X_{1}^{(i)}, \ldots, X_{I_0}^{(i)}\} \) drawn from either a typical distribution \( P_t \) or an unknown outlier distribution \( Q_f \). It notes that there may exist \( k_0 \) numbers of outlier sequences, where the integer \( k_0 \in [0, \frac{T_0}{2}] \) is uncertain. As well, the notation \( X_k^{(i)} \) denotes the \( k \)-th sample in the \( i \)-th sequence. Furthermore, by comparing the empirical typical distribution \( \hat{P}_t \) with the distribution estimation \( \hat{P}(\mathcal{X}^{(i)}) \) for every \( \mathcal{X}^{(i)} \), we have the following test as

\[
\mathcal{F}(\hat{P}(\mathcal{X}^{(i)}); \hat{P}_t) \rightarrow \begin{cases} 
\mathcal{F}(\hat{P}_t; \hat{P}_t), & \mathcal{X}^{(i)} \in \mathcal{M}_t \\
\mathcal{F}(\hat{Q}_f; \hat{P}_t), & \mathcal{X}^{(i)} \in \mathcal{M}_f 
\end{cases},
\]  

(51)

where \( \mathcal{F}(f_1; f_2) \) denotes a measurement between two distribution \( f_1 \) and \( f_2 \). \( \hat{P}_t \) and \( \hat{Q}_f \) are estimations with respect to \( P_t \) and \( Q_f \). \( \mathcal{M}_t \) and \( \mathcal{M}_f \) denote the typical sequences set and the outlier sequences set, respectively.

In practice, our sequence model for outliers detection is applicable for the case in which the outlier distributions \( Q_f \) is unknown a priori, whereas the typical distribution \( P_t \) or at least the empirical distribution \( \hat{P}_t \) is known. This is rational for many practical scenarios, in which systems regularly start without any outliers and it is easy to possess sufficient information for \( P_t \). In addition, the study of such a model can apply to many applications, such as vacant channel detection in cognitive wireless networks, fraud and anomaly detection in large data sets, state monitoring in sensor networks and so on.

**B. Outlier Detection with Divergence Measures**

Considering the performance of divergence measures on distinguishing different distributions, we can use the information distances measured by divergences to detect the outliers in the above sequence model. The method of outliers detection based on the sequence model is designed as following.

We make use of the i.i.d. samples to estimate the M-I divergence between a pending sequence and the typical sequence. The M-I divergence estimation can be applicable to the outlier sequence model as a measurement for clustering. Furthermore, a clustering algorithm such as k-means can be adopted to distinguish the outlier sequences from the typical ones. The above process is more specifically summarized in Algorithm 2. Similarly, it is feasible to design the outliers detection methods with other divergence measures such as K-L divergence and Renyi divergence.

To demonstrate the divergence measures’ availability on outlier detection, we utilize the sequence model with unknown number of outliers to characterize a kind of outlier detection scenario. As an example, we
regard a binomial distribution $B(n_0, p_a)$ as the typical distribution, in which the probability is denoted as $p_i = C_i^{n_0} p_a^i (1 - p_a)^{n_0-i}$ with $n_0 = 11$ and $p_a = 0.45$. By contrast, the i.i.d. samples drawn from another $B(n_0, p_b)$ with $p_b = 0.445$ are regarded as outliers. Then, we can randomly generate a set of sample sequences, among which each sequence consists of $T_0$ i.i.d. samples drawn from either $B(n_0, p_a)$ or $B(n_0, p_b)$. In terms of the sequence model, our goal is to detect the $k_0$ outlier sequences in the set of $T_0$ sequences.

In order to illustrate the performance of M-I divergence on outlier detection, we deal with the above example by means of Algorithm 2. Besides, we also replace the ensemble estimator and M-I divergence in that algorithm with other estimators and divergences to make comparisons, as shown in Fig. 1 and Fig. 2. In our simulation, we choose the parameter $\mu = 1/2, \varpi = 1, \epsilon = 3d$ and the distance set
Fig. 2. Means and variances of AUC with respect to different sample size in the example with sequences number $T_0 = 200$, outlier sequences number $k_0 = 20$ and the number of experiments $N_{T_0} = 100$.

**Algorithm 2** Outlier Sequences Detection with M-I divergence

**Input:** Pending sequences $\{X_1^{(i)}, \ldots, X_{T_0}^{(i)}\}$ for $i = 1, \ldots, T_0$, the typical sequence $\{Y_1, \ldots, Y_{T_0}\}$ obeying a known empirical distribution $\hat{P}_t$, the parameter $\mu$, $\varpi$

**Output:** The results of the outlier detection, $X^{(i)} \in M_f$

1: Divide $T_0$ into two parts: $M_0 \leftarrow \mu T_0$ ($0 < \mu < 1$), $N_0 \leftarrow T_0 - M_0$

2: for all $i \in [1, T_0]$ do

3: $\hat{D}_{\omega,i}(X^{(i)} || Y)$, $\hat{D}_{\omega,i}(Y || X^{(i)}) \leftarrow$ calculate the estimator of M-I divergence between $\{Y_1, \ldots, Y_{M_0}\}$ and $\{X_1^{(i)}, \ldots, X_{T_0}^{(i)}\}$ as well as the estimator of M-I divergence between $\{X_1^{(i)}, \ldots, X_{M_0}\}$ and $\{Y_1, \ldots, Y_{T_0}\}$ respectively, according to Algorithm 1.

4: $\hat{D}_{\omega,i} \leftarrow \{\hat{D}_{\omega,i}(X^{(i)} || Y) + \hat{D}_{\omega,i}(Y || X^{(i)})\}/2$

5: end for

6: Divide $\hat{D}_{\omega,i}$ into the normal set $\hat{M}_f$ or the outlier set $\hat{M}_f \leftarrow$ select a clustering algorithm such as k-means.

7: $X^{(i)} \in M_f \leftarrow \hat{D}_{\omega,i} \in \hat{M}_f$

{\tilde{d}_l = l; l = 1, 2} for the weighted ensemble estimator of M-I divergence. As well, the weight window is set to $\tilde{d} = 1$ in kernel estimator, which is used to estimate the discrete distribution in K-L divergence, Renyi divergence (with $\alpha = 1/2$) and M-I divergence (with $\varpi = 1$).

From Fig. 1, it is seen that M-I divergence outperforms K-L divergence and Renyi divergence by using
the same estimator, which matches the inequality property well. Besides, this experiment shows that M-I divergence performs better by using weighted ensemble estimator than other estimators, owing to the convergence improvement. Moreover, due to the smaller reduction in the convergence term with large samples, the kernel estimator is close to the ensemble estimator for M-I divergence.

The Fig. 2 shows that the result of outliers detection tends to be more precise as sample size increasing for M-I and K-L divergence estimated by the ensemble or kernel estimator. However, that is not dramatically improved for Renyi and M-I divergence with plug-in estimator, which may result from the small distinction between the typical distribution $B(n_0, p_a)$ and the outlier distribution $B(n_0, p_b)$. In short, it still illustrates that M-I divergence can distinguish two closing distributions more clearly rather than K-L divergence and Renyi divergence.

V. Conclusion

In this paper, we investigated the information distance problem and proposed a parametric information divergence, i.e., M-I divergence, which measures the distinction between two discrete distributions, similar to K-L divergence and Renyi divergence. Furthermore, M-I divergence has its own dramatic properties on amplifying the distance between adjacent distributions while maintaining enough gap between two nonadjacent ones. This makes M-I divergence as a promising decision making tool for the statistical big data analysis. We have investigated several fundamental properties of M-I divergence, and proposed a multidimensional kernel estimator with a weight window to estimate probability distributions in M-I divergence. Furthermore, we also presented a M-I divergence estimation algorithm by means of the weighted ensemble estimator with the window kernel. In addition, we have investigated the performance of M-I divergence on decision making of classification or clustering and applied it to design an algorithm about the outlier detection problem. In the future, we plan to investigate a parameter selection method for M-I divergence and design algorithms for other practical applications in big data.

APPENDIX A

PROOF OF THEOREM 2

Define $f(x) = e^{\alpha x - 1}$ with $\alpha > 0$ and $x > 0$. Note that $\text{Bias}(\hat{F}_d) = \mathbb{E}[f(\hat{q}_{b_0}(X)) - f(q(X))] + \mathbb{E}[f(q(X)) - f(\hat{q}(X))]$. In order to find bounds for these terms, the Taylor series expansion of $f(\hat{q}_{b_0}(X))$
Lemma 1. Let $a$ or $\bar{p}$ be a realization of the p.m.f $p$ independent of the window kernel estimators $\bar{q}_{\theta_0}$ and $\bar{p}_{\theta_0}$. As well, $p.m.f p$ and $q$ are on the same support $\mathbb{U} = [a_1, \ldots, a_L]^d$. Then, for a subscript $z$ denoting $p$ or $q$, we have

$$\tilde{c}_z(X) = \sum_{i=1}^{d} \tilde{c}_{z, i, d}(X) \left( \frac{K}{M} \right)^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M^2} \right),$$

(54a)

$$\mathbb{E}[c_z^m(X)] = \left( \sum_{i=1}^{d} \tilde{c}_{z, i, d}(X) \left( \frac{K}{M} \right)^{i/d} \right)^m + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right),$$

(54b)

where $K = \Delta \sqrt{M}$ with $\Delta = \left( \frac{2 \bar{d} + 1}{L} \right)^d \sqrt{M}$, $\tilde{c}_p(X)$ and $\tilde{c}_q(X)$ denote $\{\bar{p}_{\theta_0}(X) - \bar{p}(X)\}$ and $\{\bar{q}_{\theta_0}(X) - \bar{q}(X)\}$ respectively, as well as, $\hat{c}_{z, i, d}(X)$ is a function of $X$ and $d$, $\hat{d}_{z, i, d}$ is a function of $d$. 

\[
\begin{align*}
\mathbb{P}(\hat{q}(x_i) = \frac{\hat{U}_{d,q}(x_i)}{V_d}) = \sum_{j=1}^{M} I(y_j \in U_{d,x_i})/M V_d,
\end{align*}
\]
Proof.: As far as \( \hat{c}_p(X) \) is concerned, it is easy to see
\[
\hat{c}_p(X) = \hat{p}_{\tilde{s}_0}(X) - \tilde{p}(X)
\]
\[
= \frac{1}{N} \sum_{k=1}^{N} \left\{ \sum_{x_j \in U} W(\tilde{s}_0, X, x_j) I(x_k = x_j) - \frac{I(x_k \in U_d \setminus x)}{V_d} \right\}
\]
\[
= \frac{1}{N} \sum_{k=1}^{N} \left\{ I(x_k = x) - \frac{I(x_k \in U_d \setminus x)}{V_d} \right\} - \hat{s}_0 \left\{ \frac{1}{N} \sum_{k=1}^{N} \left\{ \frac{\sum_{x_j \in U_d \setminus x} I(x_k = x_j)}{V_d - 1} - I(x_k = x) \right\} \right\}
\]
\[
= \hat{p}(X) - \frac{\hat{U}_{d,p}(X)}{V_d} + O(\hat{s}_0),
\]
where \( \hat{U}_{d,p}(X) = \frac{1}{M} \sum_{k=1}^{M} I(x_k \in U_d \setminus x) \).

Assume that the continuous probability density function \( \hat{f}_p(x) \) has continuous partial derivatives of order \( d \). By use of Taylor series expansion, we can easily have the integral with respect to \( \hat{f}_p \) in the integral range \( B_{d,x} \) as
\[
\hat{U}_{d,f_p}(x) = \int_{B_{d,x}} \hat{f}_p(z) dz
\]
\[
= \hat{f}_p(x) V_{d,f_p}(x) + \sum_{i=1}^{d} \hat{c}_{i,d}(x) V_{d,f_p}^{1+1/d}(x) + o(V_{d,f_p}^2(x)),
\]
where \( V_{d,f_p}(x) = \int_{B_{d,x}} dz \) is the volume of set \( B_{d,x} \) and \( \hat{c}_{i,d} \) depends on \( d \) and \( \hat{f}_p \).

Let the continuous set \( B_{d,x} = \{ x : x^u \in (x^u_{i-d-1}, x^u_{i+d}) \} \) \( (u \in \{1, \ldots, d\} \) denotes \( u \)-th dimension \) correspond to the discrete set \( U_{d,x} = \{ x_j : |x^u_j - x_j| \leq \tilde{d}, x_j \in U \} \), which means \( V_{d,f_p}(x) = \int_{B_{d,x}} dz = V_d \). Then, \( \hat{f}_p(x) \) fulfills the following conditions,
\[
\left\{ \begin{array}{l}
\int_{x_{i-1}}^{x_i} \hat{f}_p(z) dz = \hat{p}(x_i) \\
\hat{f}_p(x_i) = \hat{p}(x_i),
\end{array} \right.
\]
which implies that \( \hat{U}_{d,f_p}(x_i) = \int_{B_{d,x}} \hat{f}_p(z) dz = \hat{U}_{d,p}(x_i) \).

According to the Eq. (56), it is easy to see that the \( \hat{U}_{d,p}(X) \) can be expanded as ,
\[
\hat{U}_{d,p}(X) = \int_{B_{d,x}} \hat{f}_p(z) dz
\]
\[
= \hat{p}(X) V_d + \sum_{i=1}^{d} \hat{c}_{i,d}(X) V_d^{1+1/d} + o\left(V_d^2\right),
\]
where \( V_d = (2\tilde{d} + 1)^d = \frac{K}{M} L^d \). Considering Remark 4, namely \( \tilde{s}_0 = O\left(\frac{1}{M}\right) \), and Eq. (55), it can be readily seen that
\[
\hat{c}_p(X) = \sum_{i=1}^{d} \hat{c}_{e,p,i,d}(X) \left(\frac{K}{M}\right)^{i/d} + o\left(\frac{K}{M}\right) + O\left(\frac{1}{M}\right).
\]
Furthermore, according to the binomial theorem, we have
\[
\mathbb{E}[\hat{e}_p^m(X)] = \mathbb{E}\left\lbrace \left[ \sum_{i=1}^{d} \hat{c}_{i,p,i,d}(X) \left( \frac{K}{M} \right)^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right) \right]^m \right\rbrace
\]
(60)
\[
= \left( \sum_{i=1}^{d} \hat{c}_{i,p,i,d}(X) \left( \frac{K}{M} \right)^{i/d} \right)^m + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right)
\]
Similarly, \( \hat{e}_q(X) \) and \( \mathbb{E}[\hat{e}_q^m(X)] \) can also be derived. Therefore, it is apparent that Lemma 1 has been testified.

**Lemma 2.** For a \( d \)-dimension variable \( X \) which denotes a realization of p.m.f \( p \) independent of the window kernel estimators \( \tilde{p}_{\delta_0} \) and \( \tilde{q}_{\delta_0} \), we have
\[
\tilde{h}(X) = \sum_{i=1}^{d} \hat{c}_{i,h,i,d}(X) \left( \frac{K}{M} \right)^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right),
\]
(61a)
\[
\mathbb{E}[\tilde{h}(X)] = \sum_{i=1}^{d} c_{i,h,i,d}(X) \left( \frac{K}{M} \right)^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right),
\]
(61b)
where \( \tilde{h}(X) \) denotes \( \frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)} - \frac{\tilde{q}(X)}{\tilde{p}(X)} \), \( \hat{c}_{i,h,i,d}(X) \) is a function of \( \hat{d} \), \( p \) and \( q \), as well as, \( \hat{c}_{i,h,i,d}(X) \) is a function of \( X \), \( \hat{d} \), \( p \) and \( q \).

**Proof.** By expanding the \( \frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)} \)-around \( \tilde{q}(X) \) and \( \tilde{p}(X) \), we can readily have
\[
\tilde{h}(X)
= \frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)} \tilde{q}(X) - \frac{\tilde{q}(X)}{\tilde{p}(X)} \tilde{p}(X) + \frac{\tilde{q}(X)}{\tilde{p}(X)} \tilde{p}(X)
\]
(62)
\[
- \frac{\tilde{q}(X)}{\tilde{p}(X)} \tilde{p}(X)
\]
where \( \hat{c}_{p}(X) \) and \( \hat{c}_{q}(X) \) denote \( \{\tilde{p}_{\delta_0}(X) - \tilde{p}(X)\} \) and \( \{\tilde{q}_{\delta_0}(X) - \tilde{q}(X)\} \), respectively.

According to Lemma 1, it is not difficult to see that
\[
\tilde{h}(X)
= \sum_{i=1}^{d} \hat{c}_{h_1,i,d}(X) \left( \frac{K}{M} \right)^{i/d} + \left( \sum_{i=1}^{d} \hat{c}_{h_2,i,d}(X) \left( \frac{K}{M} \right)^{i/d} \right)^2 + \left( \sum_{i=1}^{d} \hat{c}_{h_3,i,d}(X) \left( \frac{K}{M} \right)^{i/d} \right)^3
\]
(63)
\[
+ o\left( \left( \sum_{i=1}^{d} \hat{c}_{h_4,i,d}(X) \left( \frac{K}{M} \right)^{i/d} \right)^3 \right) + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right)
\]
\[
= \sum_{i=1}^{d} \hat{c}_{h,i,d}(X) \left( \frac{K}{M} \right)^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right).
\]
Furthermore, by applying the binomial theorem, we have
\[
\mathbb{E}[\hat{h}^t(X)] = \left( \sum_{i=1}^{d} \hat{c}_{h,i,d}(\frac{K}{M})^{i/d} \right)^t + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right),
\]
which can indicate that the lemma is proved.

According to Lemma 2 and Eq. (52a), it is readily seen that
\[
\mathbb{E} \left[ f\left( \frac{\tilde{q}_{h_0}(X)}{p_{h_0}(X)} \right) - f\left( \frac{\tilde{q}(X)}{p(X)} \right) \right] = \mathbb{E} \left[ \sum_{i=1}^{d} \hat{c}_{h,i,d}(X)\hat{h}^i(X) + o\left( \hat{c}_{h,i,d}(X)\hat{h}^2(X) \right) \right]
\]
\[
= \sum_{i=1}^{d} \hat{c}_{h,i,d}(\frac{K}{M})^{i/d} + \left( \sum_{i=1}^{d} \hat{c}_{h,i,d}(\frac{K}{M})^{i/d} \right)^2 + o\left( \left( \sum_{i=1}^{d} \hat{c}_{h,i,d}(\frac{K}{M})^{i/d} \right)^2 \right) + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right)
\]
\[
= \sum_{i=1}^{d} c_{h,i,d}(\frac{K}{M})^{i/d} + o\left( \frac{K}{M} \right) + O\left( \frac{1}{M} \right). \tag{65}
\]

**Lemma 3.** Let a \( d \)-dimension variable \( X \) be a realization of p.m.f \( p \) independent of \( \bar{p} \) and \( \bar{q} \) mentioned in Eq. (53). Then it can be given that
\[
\mathbb{E}[\bar{e}_p^m(X)] = \mathbb{E}[\{(\bar{p}(X) - p(X))^m\}]
\]
\[
= \sum_{i=1}^{d} \bar{c}_{e_p,i,d}(\frac{K}{M})^{i/d} + o\left( \frac{K}{M} \right) + o\left( \frac{1}{\sqrt{M}} \right) + o\left( \frac{1}{K} \right), \tag{66a}
\]
\[
= \sum_{i=1}^{d} \bar{c}_{e_q,i,d}(\frac{K}{M})^{i/d} + o\left( \frac{K}{M} \right) + o\left( \frac{1}{\sqrt{M}} \right) + o\left( \frac{1}{K} \right), \tag{66b}
\]
where \( \bar{c}_{e_p,i,d} \) and \( \bar{c}_{e_q,i,d} \) are functions of \( \hat{d} \).

**Proof.** Define \( U_{\hat{d},p}(X) = \mathbb{E}\left[ \frac{1}{M} \sum_{i=1}^{M} I(x_i \in U_{\hat{d},X}) \right] = \sum_{x_i \in U_{\hat{d},X}} p(x_i) \). On the one hand, for \( \hat{e}_p(X) = \bar{p}(X) - \frac{U_{\hat{d},p}(X)}{V_{\hat{d}}} \), it is readily seen that
\[
\mathbb{E}[\hat{e}_p(X)] = \mathbb{E}\left[ \frac{\hat{U}_{\hat{d},p}(X)}{V_{\hat{d}}} - \frac{U_{\hat{d},p}(X)}{V_{\hat{d}}} \right] = 0. \tag{67}
\]
Furthermore, we have
\[
\operatorname{Var}\left( \frac{\hat{U}_{d,p}(X)}{V_d} \right) = \frac{\mathbb{E}[\sum_{i=1}^{M} I_{(X_i \in \mathcal{U}_{d,X})}]}{M^2V_d^2} + \frac{\sum_{i=1}^{M} \sum_{j \neq i}^{M} I_{(X_i \in \mathcal{U}_{d,X})} I_{(X_j \in \mathcal{U}_{d,X})}}{M^2V_d^2} - \frac{U_{d,p}^2(X)}{V_d^2} \tag{68}
\]
which implies \(\mathbb{E}[\hat{\varepsilon}_p^2(X)] = O(1/M)\).

By using Chebyshev’s inequality, we get
\[
P \left\{ \left| \frac{\hat{U}_{d,p}(X)}{V_d} - \frac{U_{d,p}(X)}{V_d} \right| \geq \varepsilon \right\} \leq \frac{\operatorname{Var}\left( \frac{\hat{U}_{d,p}(X)}{V_d} \right)}{\varepsilon^2}, \tag{69}
\]
where \(\hat{U}_{d,p}(X) = \frac{1}{M} \sum_{k=1}^{M} I_{(X_k \in \mathcal{U}_{d,X})}\). Let \(\varepsilon = \left(\frac{1}{K}\right)^{\eta/2}\) with some fixed \(\eta \in (\frac{2}{3}, 1)\). In that case, we have \(\operatorname{Var}(\hat{\varepsilon}_p)/\varepsilon^2 = O\left(\frac{K^\eta}{M}\right)\). Thus, it is derived that
\[
\hat{\varepsilon}_p(X) = \hat{\varepsilon}_p(X) \{ P\{ |\hat{\varepsilon}_p(X)| < \varepsilon \} + P\{ |\hat{\varepsilon}_p(X)| \geq \varepsilon \} \}
= \hat{\varepsilon}_p(X) I_{\{|\hat{\varepsilon}_p(X)| < \varepsilon \}} P\{ |\hat{\varepsilon}_p(X)| < \varepsilon \} + \hat{\varepsilon}_p(X) I_{\{|\hat{\varepsilon}_p(X)| \geq \varepsilon \}} P\{ |\hat{\varepsilon}_p(X)| < \varepsilon \} + O\left(\frac{K^\eta}{M}\right) \tag{70}
\]
\[
< \varepsilon + O\left(\frac{K^\eta}{M}\right) = O\left(\left(\frac{1}{K}\right)^{\eta/2}\right) + O\left(\frac{K^\eta}{M}\right).
\]
Furthermore, it is readily seen that
\[
\mathbb{E}[\hat{\varepsilon}_p^m(X)] = \mathbb{E}[\{ I_{m=2} \hat{\varepsilon}_p^2(X) + I_{m \geq 3} \hat{\varepsilon}_p^m(X) \}]
= I_{m=2} O\left(\frac{1}{M}\right) + I_{m \geq 3} O\left(\left(\frac{1}{K}\right)^{m\eta/2}\right) \tag{71}
\]
\[
= I_{m=2} O\left(\frac{1}{M}\right) + I_{m \geq 3} O\left(\frac{1}{K}\right).
\]
Similarly, for \(\mathbb{E}[\hat{\varepsilon}_p^n(X)]\), we get the same result as \(\mathbb{E}[\hat{\varepsilon}_p^m(X)]\).

On the other hand, it is not difficult to see that the relationship between \(U_{d,p}(X)\) and \(p(X)\) is similar to \(\hat{U}_{d,p}(X)\) and \(\hat{p}(X)\) in Eq. (58). Thus, it is easily seen that
\[
\hat{\varepsilon}_p(X) = \frac{U_{d,p}(X)}{V_d} - p(X)
= \sum_{i=1}^{d} \hat{c}_{i,d}(X) \left(\frac{K}{M}\right)^{i/d} + o\left(\frac{K}{M}\right). \tag{72}
\]
Furthermore, we have
\[
\mathbb{E}[\hat{\varepsilon}_p^m(X)] = \left(\sum_{i=1}^{d} \hat{c}_{p,i,d} \left(\frac{K}{M}\right)^{i/d}\right)^m + o\left(\frac{K}{M}\right). \tag{73}
\]
As for \( \tilde{e}_p(X) \), by applying the binomial theorem and Cauchy-Schwartz inequality, we have

\[
\mathbb{E}[\tilde{e}_p^m(X)] = \mathbb{E}[\{\tilde{e}_p(X) + \tilde{e}_p(X)\}^m] = \mathbb{E}\left[\sum_{j=0}^{m} \tilde{a}_{p,j} \tilde{e}_p(X)^j \tilde{e}_p^{m-j}(X)\right] \\
\leq \sum_{j=0}^{m} \tilde{a}_{p,j} \mathbb{E}[\tilde{e}_p^j(X)] \mathbb{E}[\tilde{e}_p^{m-j}(X)] \\
= \sqrt{\mathbb{E}[\tilde{e}_p^2(X)]} + \sum_{j=1}^{m} \tilde{a}_{p,j} \sqrt{\mathbb{E}[\tilde{e}_p^j(X)] \mathbb{E}[\tilde{e}_p^{m-j}(X)]} \\
= \sum_{i=1}^{d} \tilde{c}_{p,i} \mathbb{E}[\tilde{h}_i(X)]^{i/d} + o\left(\frac{K}{M}\right) + o\left(\frac{1}{M}\right) + o\left(\frac{1}{K}\right),
\]

where \( \tilde{a}_{p,j} \) is the binomial coefficient.

Similarly, we can derive \( \mathbb{E}[\tilde{e}_q^n(X)] \), as well as, the proof of Lemma 3 is completed.

By expanding the \( \frac{\hat{q}(X)}{\hat{p}(X)} \) around \( q(X) \) and \( p(X) \), we can make use of Lemma 3 to derive \( \hat{h}(X) = \frac{\hat{q}(X)}{\hat{p}(X)} - \frac{\hat{q}(X)}{\hat{p}(X)} \) and \( \mathbb{E}[\hat{h}(X)] \), similar to Lemma 2. Furthermore, using the same way as Eq. (65), we can easily see that

\[
\mathbb{E}\left[f\left(\frac{\tilde{q}(X)}{\tilde{p}(X)}\right) - f\left(\frac{q(X)}{p(X)}\right)\right] \\
= \mathbb{E}\left[\sum_{i=1}^{d} \tilde{c}_{h,i} \mathbb{E}[\tilde{h}_i(X)]^{i/d} + o\left(\frac{K}{M}\right) + o\left(\frac{1}{K}\right)\right].
\]

Therefore, by combining Eq. (65) and Eq. (75), the proof of Theorem 2 can be completed.

**APPENDIX B**

**PROOF OF THEOREM 3**

For the function \( f(x) = e^{\alpha x^{-1}} \) with \( \alpha > 0 \) and \( x > 0 \), we can do a Taylor series expansion of \( f\left(\frac{\tilde{q}_{\alpha}(X)}{\tilde{p}_{\alpha}(X)}\right) \) around \( \mathbb{E}\left[\tilde{q}_{\alpha}(X)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X)] \) as following

\[
f\left(\frac{\tilde{q}_{\alpha}(X)}{\tilde{p}_{\alpha}(X)}\right) = \sum_{i=0}^{2} \frac{f^{(i)}\left(\mathbb{E}\left[\tilde{q}_{\alpha}(X)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X)]\right)}{i!} \tilde{g}(X) + \frac{1}{6}f^{(3)}(\xi_X)\tilde{g}^3(X),
\]

where \( \xi_X \in \left(\mathbb{E}\left[\tilde{q}_{\alpha}(X)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X)]\right) \) comes from the mean value theorem, and \( \tilde{g}(X) \) denotes \( \frac{\tilde{q}_{\alpha}(X)}{\tilde{p}_{\alpha}(X)} - \mathbb{E}\left[\tilde{q}_{\alpha}(X)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X)] \]. Define the operator \( \mathcal{H}(Z) = Z - \mathbb{E}(Z) \). Let

\[
a_i = \mathcal{H}\left(f\left(\mathbb{E}\left[\tilde{q}_{\alpha}(X_i)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X_i)]\right)\right),
\]

\[
b_i = \mathcal{H}\left(f\left(\mathbb{E}\left[\tilde{q}_{\alpha}(X_i)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X_i)]\right)\tilde{g}(X_i)\right),
\]

\[
b_i = \mathcal{H}\left(f\left(\mathbb{E}\left[\tilde{q}_{\alpha}(X_i)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X_i)]\right)\tilde{g}(X_i)\right) \\
= \mathcal{H}\left(\mathbb{E}\left[\tilde{q}_{\alpha}(X_i)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X_i)]\right) \tilde{g}(X_i) + \frac{1}{6}f^{(3)}(\xi_{X_i})\tilde{g}^3(X_i),
\]

where \( \xi_{X_i} \in \left(\mathbb{E}\left[\tilde{q}_{\alpha}(X_i)\right]/\mathbb{E}[\tilde{p}_{\alpha}(X_i)]\right) \) comes from the mean value theorem.
Then the variance of $\hat{F}_d$ is

$$\text{Var}(\hat{F}_d) = \mathbb{E}[(\hat{F}_d - \mathbb{E}(\hat{F}_d))^2]$$

$$= \frac{1}{N} \mathbb{E}[(a_1 + b_1 + c_1 + d_1)^2] + \frac{N - 1}{N} \mathbb{E}[(a_1 + b_1 + c_1 + d_1)(a_2 + b_2 + c_2 + d_2)],$$

which can be bounded in the following.

**Lemma 4.** For a $d$-dimension variable $X$, a realization of p.m.f $p$ independent of the window kernel estimators $\tilde{q}$ and $\tilde{p}$, it can be given that

$$\mathbb{E}[e^m_p(X)] = \mathbb{E} \left[ \left( \tilde{p} - \mathbb{E}[\tilde{p}] \right)^m \right] = o \left( \frac{1}{K} \right)$$

$$\mathbb{E}[e^n_q(X)] = \mathbb{E} \left[ \left( \tilde{q} - \mathbb{E}[\tilde{q}] \right)^n \right] = o \left( \frac{1}{K} \right)$$

where $K = \Delta \sqrt{M}$ with $\Delta = \left( \frac{2d}{L} \right)^d \sqrt{M}$, $e_p(X)$ and $e_q(X)$ denote $\{\tilde{p} - \mathbb{E}[\tilde{p}]\}$ and $\{\tilde{q} - \mathbb{E}[\tilde{q}]\}$, respectively.

**Proof.** For the $e_p(X) = \tilde{p} - \mathbb{E}[\tilde{p}]$, it is readily seen that

$$\mathbb{E}[e_p(X)] = \mathbb{E}[\tilde{p} - \mathbb{E}[\tilde{p}]] = 0.$$  

In addition, by use of the definition 3, we have

$$\text{Var}(\tilde{p}) = \mathbb{E}[\tilde{p}^2] - \mathbb{E}^2(\tilde{p})$$

$$= \frac{1}{M} \sum_{x_j \in \mathbb{U}_d} W^2(\tilde{s}_0, X, x_j)p(x_j) - \frac{1}{M} \left[ \sum_{x_j \in \mathbb{U}_d} W(\tilde{s}_0, X, x_j)p(x_j) \right]^2,$$

where $\mathbb{U}_d = \{x_j : |x^u_j - X^u| \leq d, x_j \in \mathbb{U}\}$. Consequently, it is evident to see that $\mathbb{E}[e^2_p(X)] = O(1/M)$.

$$e_p(X)$$

$$= e_p(X) \left\{ P \{ |e_p(X) | < \varepsilon \} + P \{ |e_p(X) | \geq \varepsilon \} \right\}$$

$$= e_p(X) \left\{ P \{ |e_p(X) | < \varepsilon \} \right\} + O \left( \frac{K^\eta}{M} \right)$$

$$< \varepsilon + O \left( \frac{K^\eta}{M} \right) = O \left( \left( \frac{1}{K} \right)^{\eta/2} + O \left( \frac{K^\eta}{M} \right) \right).$$
Consequently, we get

\[
\mathbb{E}[e_p^m(X)] = \mathbb{E}[I_{(m=2)}e_p^2(X) + I_{(m\geq 3)}e_p^m(X)]
\]

\[
= I_{(m=2)}O\left(\frac{1}{M}\right) + I_{(m\geq 3)}O\left(\left(\frac{1}{K}\right)^{m/2}\right)
\]

\[
= I_{(m=2)}O\left(\frac{1}{M}\right) + I_{(m\geq 3)}o\left(\frac{1}{K}\right).
\]

Similarly, it can be proved that \(\mathbb{E}[e_q^n(X)]\) has the same result as \(\mathbb{E}[e_p^m(X)]\).

By using a Taylor series expansion of \(1/\tilde{p}_{\delta_0}(X)\) around \(\mathbb{E}[\tilde{p}_{\delta_0}(X)]\), we have

\[
\mathbb{E}\left[\frac{1}{\tilde{p}_{\delta_0}(X)}\right] = \mathbb{E}\left[\frac{1}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]}\right] - e_p(X) + \frac{e_p^2(X)}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} + o\left(e_p^2(X)\right)
\]

where \(e_p(X)\) denotes \(\{\tilde{p}_{\delta_0}(X) - \mathbb{E}[\tilde{p}_{\delta_0}(X)]\}\), and \(\tilde{\zeta}_{p,x} \in (\mathbb{E}[\tilde{p}_{\delta_0}(X)],\tilde{p}_{\delta_0}(X))\). Since the \(p\) and \(q\) are independent, it is easily to see that

\[
\mathbb{E}\left[\frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)}\right] = \mathbb{E}[\tilde{q}_{\delta_0}(X)]\mathbb{E}\left[\frac{1}{\tilde{p}_{\delta_0}(X)}\right] = \frac{\mathbb{E}[\tilde{q}_{\delta_0}(X)]}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} + o\left(e_p^2(X)\right).
\]

What is more, by expanding the \(\tilde{q}_{\delta_0}(X)/\tilde{p}_{\delta_0}(X)\) around \(\mathbb{E}[\tilde{q}_{\delta_0}(X)]\) and \(\mathbb{E}[\tilde{p}_{\delta_0}(X)]\), we have

\[
\tilde{g}(X)
\]

\[
= \frac{e_q(X)}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} - \frac{\mathbb{E}[\tilde{q}_{\delta_0}(X)]}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} e_p(X) + \frac{e_q(X)e_p(X)}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} + \frac{\mathbb{E}[\tilde{q}_{\delta_0}(X)]}{\mathbb{E}[\tilde{p}_{\delta_0}(X)]} e_p^2(X) + o(e_p^2(X) + e_q(X)e_p^2(X)),
\]

In addition, by applying the Cauchy-Schwartz inequality and Lemma 4, it is readily seen that

\[
|\mathbb{E}[e_p^m(X)e_q^n(X)]| \leq I_{\{m \geq 1, n \geq 1\}}\sqrt{\mathbb{E}[e_p^{2m}(X)]\mathbb{E}[e_q^{2n}(X)]} + \{I_{\{m>1, n=0\}} + I_{\{m=0, n>1\}}\}|\mathbb{E}[e_p^m(X)e_q^n(X)]| + \{I_{\{m=1, n=0\}} + I_{\{m=0, n=1\}}\}|\mathbb{E}[e_p^m(X)e_q^n(X)]| = o\left(\frac{1}{\sqrt{M}}\right) + o\left(\frac{1}{K}\right),
\]

where \(m > 0\) and \(n > 0\) are integers.

Therefore, by applying the multinomial theorem to Eq. (85), it is apparent that

\[
\mathbb{E}[\tilde{g}(X)] = \mathbb{E}\left\{\frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)} - \mathbb{E}\left[\frac{\tilde{q}_{\delta_0}(X)}{\tilde{p}_{\delta_0}(X)}\right]\right\} = o\left(\frac{1}{\sqrt{M}}\right) + o\left(\frac{1}{K}\right),
\]

(87)
According to Eq. (87) and Eq. (77), we have
\[
\mathbb{E}[(a_1 + b_1 + c_1 + d_1)^2] = \mathbb{E}[a_1^2] + o(1) = c_N \left( \mathbb{E}\left[ \frac{q_{s_0}(X_i)}{p_{s_0}(X_i)} \right] \right) + o(1).
\]
(88)

Moreover, due to the independent \( X_1 \) and \( X_2 \), it can be readily seen that \( \mathbb{E}[(a_1 + b_1 + c_1 + d_1)(a_2 + b_2 + c_2 + d_2)] = 0 \). Therefore, we have
\[
\text{Var}(\hat{F}_d) = \frac{1}{N} \left[ c_N \left( \mathbb{E}\left[ \frac{q_{s_0}(X_i)}{p_{s_0}(X_i)} \right] \right) + o(1) \right] = O\left( \frac{1}{N} \right),
\]
(89)

which indicates that Theorem 3 is proved.

**APPENDIX C**

**THE MSE CONVERGENCE OF M-I DIVERGENCE ESTIMATION**

According to Eq. (45) and Taylor series expansion, we have
\[
\hat{F}_d - F_\varpi(P \parallel Q) = \frac{1}{N} \sum_{i=1}^{N} \left\{ e^{\frac{\mu_s(X_i)}{q_s(X_i)}} - e^{\frac{\mu(X_i)}{q(X_i)}} \right\} + \left\{ \frac{1}{N} \sum_{i=1}^{N} e^{\frac{\mu_s(X_i)}{q_s(X_i)}} - \sum_{x_j \in U} p(x_j) e^{\frac{\mu(x_j)}{q(x_j)}} \right\}
\]
(90)

\[
= \frac{1}{N} \sum_{i=1}^{N} \left\{ e^{\frac{\mu_s(X_i)}{q_s(X_i)}} - \sum_{x_j \in U} p(x_j) e^{\frac{\mu(x_j)}{q(x_j)}} \right\}
\]

Considering Remark 3 and the law of large numbers, it is easy to see that \( \hat{F}_d - F_\varpi(P \parallel Q) \to 0 \). Therefore, we have
\[
\hat{F}_\lambda - F_\varpi(P \parallel Q) = \sum_{l \in I} \lambda_l [\hat{F}_d - F_\varpi(P \parallel Q)] \to 0,
\]
(91)

which equally means \( \hat{F}_\lambda / F_\varpi(P \parallel Q) \to 1 \).

Additionally, in virtue of corollary 3 and the definition of MSE, it is readily seen that
\[
\mathbb{E} \left\{ \left[ \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right]^2 \right\} = \text{MSE}(\hat{F}_\lambda) / F_\varpi^2(P \parallel Q) = O(I^{-1}),
\]
(92)

where \( \hat{F}_\lambda \) is the optimal ensemble estimation of \( F_\varpi(P \parallel Q) \), and \( F_\varpi(P \parallel Q) < \infty \).

Therefore, by using the Taylor series expansion of \( \log(x) \) around \( x = 1 \), we have
\[
\text{MSE}(\hat{D}_\varpi(P \parallel Q))
= \mathbb{E} \left\{ \left[ \frac{\log \hat{F}_\lambda}{F_\varpi(P \parallel Q)} \right]^2 \right\}
= \mathbb{E} \left\{ \left[ \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right] - \frac{1}{2} \left( \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right)^2 + o\left( \left( \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right)^2 \right) \right\}
= \mathbb{E} \left\{ \left[ \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right]^2 + o\left( \left( \frac{\hat{F}_\lambda}{F_\varpi(P \parallel Q)} - 1 \right)^2 \right) \right\} = O(I^{-1}),
\]
(93)

which proves Eq. (50).
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