A Test for Independence Via Bayesian Nonparametric Estimation of Mutual Information

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Abstract

Mutual information is a well-known tool to measure the mutual dependence between variables. In this paper, a Bayesian nonparametric estimation of mutual information is established by means of the Dirichlet process and the k-nearest neighbor distance. As a direct outcome of the estimation, an easy-to-implement test of independence is introduced through the relative belief ratio. Several theoretical properties of the approach are presented. The procedure is investigated through various examples where the results are compared to its frequentist counterpart and demonstrate a good performance.

Keywords: Dirichlet process, k-nearest neighbor distance, Mutual information, Relative belief inferences, Test for independence.

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1 Introduction

The assumption of independence is common in many fields such as statistics, data mining, machine learning and signal processing (Shimizu and Kano, 2003; Fernandez, 2010; Darrell et al., 2015). If this assumption is violated, the risk of having errors in the outcomes is increased. Thus, it is of particular importance to check this assumption.

A well-known tool to measure the mutual dependence between variables is the mutual information (Cover and Thomas, 2006). More precisely, let $X = (X_1, \cdots, X_d)$ be a random vector with joint continuous distribution function $F$ and marginal continuous distribution functions $F_1, \cdots, F_d$. Then mutual information between $X_1, \cdots, X_d$ is defined as

$$MI(F) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1, \ldots, x_d) \log \frac{f(x_1, \ldots, x_d)}{f(x_1) \cdots f(x_d)} \, dx_1 \cdots dx_d,$$

where $f(x_1, \cdots, x_d)$ and $f(x_i)$ denote, respectively, the probability density functions of $F$ and $F_i$, $i = 1, \ldots, d$. Note that, throughout this paper, $\log(\cdot)$ denotes the natural logarithm. Clearly, (1) is the Kullback-Leibler of $F$ from the product of $F_i$'s and so it is non-negative. After simplification, (1) can be written as

$$MI(F) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1, \ldots, x_d) \log f(x_1, \ldots, x_d) \, dx_1 \cdots dx_d - \sum_{i=1}^{d} \int_{-\infty}^{\infty} f(x_i) \log f(x_i) \, dx_i$$

$$= -H(F) + \sum_{i=1}^{d} H(F_i),$$

where $H(F)$ and $H(F_i)$ denote, respectively, the entropy of $F$ and $F_i$. Accordingly, the mutual independence between $X_1, \cdots, X_d$ can be tested by checking the hypothesis $\mathcal{H}_0 : MI(F) = 0$. Thus, from (2), to construct a test of independence via mutual information, it is essential to develop an efficient estimator for $H(F)$ and $H(F_i)$. There have been plentiful attempts to estimate the entropy but most of them are related to the univariate (marginal) entropy estimation. See for example, Vasicek (1976), Ebrahimi et al. (1994), Alizadeh Noughabi (2010), Alizadeh Noughabi and Alizadeh Noughabi (2013) and Al-Omari (2014, 2016). Also, Al-Labadi et al. (2019d) proposed an efficient Bayesian counterpart
of Vasicek’s estimator. For the multivariate (joint) entropy estimation, some frequentist procedures have been offered in the literature; see, for instance, Kozachenko and Leonenko (1987), Misra et al. (2010), Sricharan and Hero (2012), Sricharan et al. (2013), Gao et al. (2016), Berrett et al. (2019a), Ba and Lo (2019) and the references therein. Among several estimators, due to its simplicity, Kozachenko and Leonenko (1987) (KL) estimator is the most common one. Let $X_1, \ldots, X_n$ be $n$ independent random vectors each having the continuous $d$-variate cdf $F$ and let, for $i = 1, \ldots, n$, $\rho_i = \min \{ ||X_i - X_j||, j \in \{1, \ldots, n\} \setminus \{i\} \}$, where $||\cdot||$ denotes the Euclidean norm on $\mathbb{R}^d$ and $A \setminus B$ denotes the set of elements in $A$ but not in $B$. Then, the KL estimator is given by

$$H_{KL}^n = \frac{d}{n} \sum_{i=1}^{n} \log \rho_i + \log \left( \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2} + 1)} \right) + \gamma + \log(n - 1),$$  \hspace{1cm} (3)$$

where $\gamma = 0.5772 \cdots$ denotes Euler’s constant. Kozachenko and Leonenko (1987) showed that $H_{KL}^n$ is a consistent estimator. However, Singh et al. (2003) remarked that, in practical applications, the estimator (3) can be applied when the small values of the nearest neighbor distance $\rho_i$’s are recorded to high accuracy, which is often not the case. They improved the estimator $H_{KL}^n$ in (3) by proposing the following $k$-nearest neighbor ($k$-NN) version of KL estimator:

$$H_{k,KL}^n = \frac{d}{n} \sum_{i=1}^{n} \log R_{i,k,n-1} + \log \left( \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2} + 1)} \right) - L_{k-1} + \gamma + \log n,$$  \hspace{1cm} (4)$$

where, $L_0 = 0$, $L_j = \sum_{r=1}^{j} \frac{1}{r}$, $R_{i,k,n-1} = ||X_{(k)},i - X_i||$ and $X_{(1),i}, \ldots, X_{(k),i}, \ldots, X_{(n-1),i}$ is a reordering of $\{X_1, \ldots, X_n\} \setminus \{X_i\}$ such that $||X_{(1),i} - X_i|| \leq \cdots \leq ||X_{(k),i} - X_i|| \leq \cdots \leq ||X_{(n-1),i} - X_i||$. Singh et al. (2003) proved the asymptotic unbiasedness and consistency of $H_{k,KL}^n$. They used Monte Carlo simulations to find a suitable choice of $k$. For instance, they recommended using $k = 4$ as an optimal choice for sample sizes $n \leq 50$.

A primary application of mutual information is to build tests of independence. For example, in a recent work, Berrett and Samworth (2019b) developed a test of independence based on a weighted version of the KL estimator. Additional tests of independence that count on mutual information can be found in Wu et al. (2009), Mathew (2013) and Pethel and Hahs (2014). For other strategies of tests of independence such as copula process,
distance covariance, and etc; see, Genest and Rémillard (2004), Kojadinovic and Holmes (2009), Medovikov (2016), Belalia et al. (2017), Susam and Ucer (2018), Karvanen (2005), Meintanis and Iliopoulos (2008), Gaißer et al. (2010), and Fan et al. (2017) for a comprehensive review. Roy et al. (2019, pp. 12-15) pointed out that most of these methods suffer from a weak performance for sample sizes less than or equal to 50.

As seen earlier, there are extensive frequentist multivariate entropy estimations. On the other side, Bayesian estimation has been not received much attention. To the best knowledge of the authors, there are only two works related to test of independence that use Bayesian nonparametric (BNP) techniques. The first one, due to Filippi et al. (2016), uses Dirichlet process mixture prior on the unknown distribution of the data to present two BNP diagnostic measures for detecting pairwise dependencies that are scalable to large data sets. The second work, due to Filippi and Holmes (2017), considers Pólya tree prior to derive an explicit form of Bayes factor to state evidence for independence between pairs of random variables. Both of the previous works do not rely on entropy estimation. Thus, deriving a general BNP estimator of entropy that supports both marginal and joint entropy estimation with small systematic errors appears thought-provoking. Developing such an estimator will be the first goal of this paper. Having the estimator in hand makes it possible to construct a Bayesian test for independence. The anticipated estimator may be viewed as the BNP counterpart of (4). The Dirichlet process and relative belief ratio are utilized to build the test. As seen in the next sections, the developed test is easy-to-implement with an excellent performance particularly for small sample sizes.

The reminder of this paper is as follow. A relevant background containing some definitions and generic properties of the Dirichlet process and the relative belief ratio are reviewed in Section 2. Section 3 is a central section where a BNP estimator of mutual information is developed through estimating joint and marginal entropies. In addition, several theoretical properties of the proposed estimator are derived. It also discusses the choice of the hyperparameter of the Dirichlet process. In Section 4, a test for independence is presented as a result of the estimation of mutual information. Computational algorithms to implement the approach are outlined in Section 5. In Section 6, the pro-
cEDURE is investigated through several examples where the results are compared to its frequentist counterpart. Finally, Section 7 concludes the paper with a summary of the results. A short proof to clarify some expressions related to Section 3 is given in the Appendix.

2 Relevant Background

2.1 Dirichlet Process

The Dirichlet process, introduced by Ferguson (1973), is the most commonly used prior in BNP inferences. A remarkable collection of nonparametric inferences have been devoted to this prior. In this section, we only present the most relevant definitions and properties of this prior. Consider a space $\mathcal{X}$ with a $\sigma$-algebra $\mathcal{A}$ of subsets of $\mathcal{X}$, let $G$ be a fixed probability measure on $(\mathcal{X}, \mathcal{A})$, called the base measure, and $a$ be a positive number, called the concentration parameter. A random probability measure $P = \{P(A) : A \in \mathcal{A}\}$ is called a Dirichlet process on $(\mathcal{X}, \mathcal{A})$ with parameters $a$ and $G$, denoted by $P \sim \text{DP}(a, G)$, if for every measurable partition $A_1, \ldots, A_k$ of $\mathcal{X}$ with $k \geq 2$, the joint distribution of the vector $(P(A_1), \ldots, P(A_k))$ has the Dirichlet distribution with parameter $aG(A_1), \ldots, aG(A_k)$. Also, it is assumed that $G(A_j) = 0$ implies $P(A_j) = 0$ with probability one. Consequently, for any $A \in \mathcal{A}$, $P(A) \sim \text{beta}(aG(A), a(1 - G(A)))$, $E(P(A)) = G(A)$ and $\text{Var}(P(A)) = G(A)(1 - G(A))/(1 + a)$. Accordingly, the base measure $G$ plays the role of the center of $P$ while the concentration parameter $a$ controls the variation of $P$ around $G$.

One of the most well-known properties of the Dirichlet process is the conjugacy property. That is, when the sample $x = (x_1, \ldots, x_n)$ is drawn from $P \sim \text{DP}(a, G)$, the posterior distribution of $P$ given $x$, denoted by $P^*$, is also a Dirichlet process with concentration parameter $a + n$ and base measure

$$G_{a,n}^* = a(a + n)^{-1}G + n(a + n)^{-1}F_n,$$ (5)
where $F_n$ denotes the empirical cumulative distribution function (cdf) of the sample $x$.

Note that, $G_{a,n}^*$ is a convex combination of the base measure $G$ and the empirical cdf $F_n$. Therefore, $G_{a,n}^* \rightarrow G$ as $a \rightarrow \infty$ while $G_{a,n}^* \rightarrow F_n$ as $a \rightarrow 0$. On the other hand, by Glivenko-Cantelli theorem, when $n \rightarrow \infty$, $G_{a,n}^*$ converges to true distribution function generating the data. A guideline about choosing the hyperparameters $a$ and $G$ will be covered for the test of independence in Section 4. Following Ferguson (1973), $P \sim DP(a, G)$ can be represented as

$$P = \sum_{i=1}^{\infty} L^{-1}(\Gamma_i) \delta_{Y_i} / \sum_{i=1}^{\infty} L^{-1}(\Gamma_i), \quad (6)$$

where $\Gamma_i = E_1 + \cdots + E_i$ with $E_i \overset{i.i.d.}{\sim} \text{exponential}(1), Y_i \overset{i.i.d.}{\sim} G$ independent of the $
\Gamma_i, L^{-1}(y) = \inf\{x > 0 : L(x) \geq y\}$ with $L(x) = \int_{x}^{\infty} t^{-1} e^{-t} dt, x > 0$, and $\delta_a$ the Dirac delta measure. The series representation (6) implies that the Dirichlet process is a discrete probability measure even for the cases with an absolutely continuous base measure $G$. Note that, by imposing the weak topology, the support of the Dirichlet process could be quite large, namely, the support is the set of all probability measures whose support is contained in the support of the base measure. Recognizing the complexity when working with (6) (i.e., no closed form for the inverse of Lévy measure $L(x)$ exists), Ishwaran and Zarepour (2003) proposed the following finite representation as an efficient method to simulate the Dirichlet process. They showed that the Dirichlet process $P \sim DP(a, G)$ can be approximated by

$$P_N = \sum_{i=1}^{N} J_{i,N} \delta_{Y_i}, \quad (7)$$

where, $(J_{1,N}, \ldots, J_{N,N}) \sim \text{Dirichlet}(a/N, \ldots, a/N)$. Then $E_{P_N}(g) \rightarrow E_{P}(g)$ in distribution as $N \rightarrow \infty$, for any measurable function $g : \mathbb{R} \rightarrow \mathbb{R}$ with $\int_{\mathbb{R}} |g(x)| H(dx) < \infty$ and $P \sim DP(a, H)$. In particular, $(P_{N})_{N \geq 1}$ converges in distribution to $P$, where $P_{N}$ and $P$ are random values in the space $M_1(\mathbb{R})$ of probability measures on $\mathbb{R}$ endowed with the topology of weak convergence. To generate $(J_{i,N})_{1 \leq i \leq N}$ put $J_{i,N} = G_{i,N} / \sum_{i=1}^{N} G_{i,N}$, where $(G_{i,N})_{1 \leq i \leq N}$ is a sequence of i.i.d. gamma($a/N, 1$) random variables independent of $(Y_{i})_{1 \leq i \leq N}$. This form of approximation leads to some results in Section 3.
2.2 Relative Belief Inferences

The relative belief ratio, developed by Evans (2015), becomes a widespread measure of statistical evidence. See, for example, the work of Al-Labadi and Evans (2018), Al-Labadi et al. (2017, 2018), Al-Labadi et al. (2019a,b) and Al-Labadi et al. (2019c) for implementation of the relative belief ratio on different stimulating model checking problems. In details, let \( \{ f_\theta : \theta \in \Theta \} \) be a collection of densities on a sample space \( X \) and let \( \pi \) be a prior on the parameter space \( \Theta \). Note that the densities may represent discrete or continuous probability measures but they are all with respect to the same support measure \( d\theta \).

After observing the data \( x \), the posterior distribution of \( \theta \), denoted by \( \pi(\theta | x) \), is a revised prior and is given by the density \( \pi(\theta | x) = \pi(\theta) f_\theta(x)/m(x) \), where \( m(x) = \int_\Theta \pi(\theta) f_\theta(x) \, d\theta \) is the prior predictive density of \( x \). For a parameter of interest \( \psi = \Psi(\theta) \), let \( \Pi_\Psi \) be the marginal prior probability measure and \( \Pi_\Psi(\cdot | x) \) be the marginal posterior probability measure. It is assumed that \( \Psi \) satisfies regularity conditions so that the prior density \( \pi_\Psi \) and the posterior density \( \pi_\Psi(\cdot | x) \) of \( \psi \) exist with respect to some support measure on the range space for \( \Psi \).

The relative belief ratio for a value \( \psi \) is then defined by

\[
RB_\Psi(\psi | x) = \lim_{\delta \to 0} \frac{\Pi_\Psi(N_\delta(\psi) | x)}{\Pi_\Psi(N_\delta(\psi))},
\]

where \( N_\delta(\psi) \) is a sequence of neighborhoods of \( \psi \) converging nicely to \( \psi \) as \( \delta \to 0 \) (Evans, 2015). When \( \pi_\Psi \) and \( \pi_\Psi(\cdot | x) \) are continuous at \( \psi \), the relative belief ratio is defined by

\[
RB_\Psi(\psi | x) = \frac{\pi_\Psi(\psi | x)}{\pi_\Psi(\psi)},
\]

the ratio of the posterior density to the prior density at \( \psi \). Therefore, \( RB_\Psi(\psi | x) \) measures the change in the belief of \( \psi \) being the true value from a priori to a posteriori.

Since \( RB_\Psi(\psi | x) \) is a measure of the evidence that \( \psi \) is the true value, if \( RB_\Psi(\psi | x) > 1 \), then the probability of \( \psi \) being the true value from a priori to a posteriori is increased, consequently there is evidence based on the data that \( \psi \) is the true value. If \( RB_\Psi(\psi | x) < 1 \), then the probability of \( \psi \) being the true value from a priori to a posteriori is decreased. Accordingly, there is evidence against based on the data that \( \psi \) being the true value. For the case \( RB_\Psi(\psi | x) = 1 \) there is no evidence either way.
Obviously, $RB_\Psi(\psi_0 \mid x)$ measures the evidence of the hypothesis $H_0: \Psi(\theta) = \psi_0$. Large values of $RB_\Psi(\psi_0 \mid x) = c$ provides strong evidence in favor of $\psi_0$. However, there may also exist other values of $\psi$ that had even larger increases. Thus, it is also necessary, however, to calibrate whether this is strong or weak evidence for or against $H_0$. A typical calibration of $RB_\Psi(\psi_0 \mid x)$ is given by the strength

$$\Pi_\Psi [RB_\Psi(\psi \mid x) \leq RB_\Psi(\psi_0 \mid x) \mid x]. \quad (8)$$

The value in (8) indicates that the posterior probability that the true value of $\psi$ has a relative belief ratio no greater than that of the hypothesized value $\psi_0$. Noticeably, (8) is not a p-value as it has a very different interpretation. When $RB_\Psi(\psi_0 \mid x) < 1$, there is evidence against $\psi_0$, then a small value of (8) indicates strong evidence against $\psi_0$. On the other hand, a large value for (8) indicates weak evidence against $\psi_0$. Similarly, when $RB_\Psi(\psi_0 \mid x) > 1$, there is evidence in favor of $\psi_0$, then a small value of (8) indicates weak evidence in favor of $\psi_0$, while a large value of (8) indicates strong evidence in favor of $\psi_0$.

3 BNP Posterior of mutual information

In this section, we provide a posterior of entropy and use it in (2) to propose a posterior of mutual information.

3.1 Prior and Posterior of Entropy

Let $P_N = \sum_{i=1}^N J_{i,N} \delta_{Y_i}$ be as defined by (7), where $(J_{1,N}, \ldots, J_{N,N}) \sim \text{Dirichlet}(a/N, \ldots, a/N)$, $Y_1, \ldots, Y_N \overset{i.i.d.}{\sim} G$, and $Y_i \in \mathbb{R}^d$. The proposed $k$-NN BNP prior of entropy is defined by

$$H_{N,a,k}^{\text{post}} = \sum_{i=1}^N J_{i,N} \left( \log \left( \frac{N - 1}{k \Gamma(\frac{d}{2} + 1)} \right) - L_{k-1} + \gamma + \log k \right)$$

$$= \sum_{i=1}^N J_{i,N} T_i^{(N-1)} - L_{k-1} + \gamma + \log k, \quad (9)$$
where \(k \in \{1, \ldots, N-1\}\) and \(R_{i,k,N-1}\) is the euclidean distance between \(Y_i\) and its \(k\)-th closest neighbor. The next lemma shows the asymptotic behavior of the expectation and the variance of \(H_{N,a,k}^{pri}\), when \(N \to \infty\) and \(a \to \infty\).

**Lemma 1** Let \(G\) be a \(d\)-variate distribution and \(F \sim DP(a, G)\). Consider the \(k\)-NN BNP prior \(H_{N,a,k}^{pri}\) as defined in (9), then

i. \(E(H_{N,a,k}^{pri}) \to H(G)\), as \(N \to \infty\),

ii. \(Var(H_{N,a,k}^{pri}) \to 0\), as \(N \to \infty\) and \(a \to \infty\).

**Proof.** To prove (i), since \(J_{i,N}\) and \(T_i^{(N-1)}\) are independent, we have

\[
E(H_{N,a,k}^{pri}) = \sum_{i=1}^{N} \left( E(T_i^{(N-1)} E(J_{i,N})) - L_{k-1} + \gamma + \log k \right)
\]

Noting that \(E(J_{i,N}) = 1/N\), and \((T_i^{(N-1)})_{1 \leq i \leq N}\) are identically distributed random variables, we have

\[
E(H_{N,a,k}^{pri}) = E(T_1^{(N-1)}) - L_{k-1} + \gamma + \log k.
\]

From Singh et al. (2003), \(E(T_1^{(N-1)}) \to L_{k-1} - \gamma - \log k + H(G)\) as \(N \to \infty\), and the result follows. To prove (ii), since \(Var(J_{i,N}) = \frac{N-1}{N^2(a+1)}\) and \(Cov(J_{i,N}, J_{j,N}) = \frac{-1}{N^2(a+1)}\), we have

\[
Var(H_{N,a,k}^{pri}) = Var \left( E \left( \sum_{i=1}^{N} T_i^{(N-1)} J_{i,N} | T_1^{(N-1)}, \ldots, T_N^{(N-1)} \right) \right)
\]

\[
+ E \left( Var \left( \sum_{i=1}^{N} T_i^{(N-1)} J_{i,N} | T_1^{(N-1)}, \ldots, T_N^{(N-1)} \right) \right)
\]

\[
= Var \left( \frac{1}{N} \sum_{i=1}^{N} T_i^{(N-1)} \right) + E \left( \frac{N-1}{N^2(a+1)} \sum_{i=1}^{N} (T_i^{(N-1)})^2 \right) - \frac{2}{N^2(a+1)}
\]

\[
\times \sum_{i<j}^{N} T_i^{(N-1)} T_j^{(N-1)}
\]

\[
= \frac{1}{N} Var \left( T_1^{(N-1)} \right) + \frac{N-1}{N} Cov \left( T_1^{(N-1)}, T_2^{(N-1)} \right) + \frac{N-1}{N(a+1)} \left( E \left( T_1^{(N-1)} \right) \right)^2
\]

\[- E \left( T_1^{N-1} T_2^{N-1} \right) \] (10)
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From Singh et al. (2003), \( \text{Var} \left( T_1^{(N-1)} \right) \to Q_k + \text{Var} \left( \log g(y) \right) \), \( \text{Cov} \left( T_1^{(N-1)}, T_2^{(N-1)} \right) \to 0 \), \( \text{Cov} \left( T_1^{(N-1)}, T_2^{(N-1)} \right) \to \left[ L_{K-1} - \gamma - \log k + H(G) \right]^2 \) as \( N \to \infty \), where \( Q_k = \sum_{j=k}^{\infty} \frac{1}{j^2} \), \( g \) denotes the probability density function of \( G \) and \( y \in \mathbb{R}^d \). Hence, by letting \( N \to \infty \) in (10), we have

\[
\text{Var}(H_{N,a,k}^{\text{pri}}) \to \frac{1}{a+1} \left\{ Q_k + \text{Var} \left( \log g(y) \right) \right\}. \tag{11}
\]

Letting \( a \to \infty \), gives the proof of (ii).

The next corollary shows the asymptotic behavior of the variance of \( H_{N,a,k}^{\text{pri}} \) when \( N \to \infty \) and \( k \to \infty \).

**Corollary 2** Consider \( H_{N,a,k}^{\text{pri}} \) as defined in (9). Then, for fixed \( a \), as \( N \to \infty \) and \( k \to \infty \), we have

\[
\text{Var}(H_{N,a,k}^{\text{pri}}) \to \frac{1}{a+1} \text{Var} \left( \log g(y) \right).
\]

**Proof.** Note that \( Q_k = \sum_{j=k}^{\infty} \frac{1}{j^2} \) can be written as \( \int_0^{\infty} \frac{t}{1-e^{-kt}} \, dt \) (Abramowitz and Stegun, 1972, p. 260). Hence, by letting \( k \to \infty \) in (11), the monotone convergence theorem implies that \( Q_k \to 0 \) and the result follows.

From Corollary 2, for a fixed value of \( a \), choosing too large values of \( k \) reduces the statistical errors; however, in practical applications, for such values of \( k \), the increase of systematic errors outweighs the decrease of statistical errors (Singh et al., 2003; Kraskov et al., 2004). In Section 6, we performed a simulation study to assess the effect of different values of \( k \) on the behavior of the systematic errors. As a result, we recommend choosing \( k = 3 \) in the BNP procedure.

Now, by the conjugacy property of the Dirichlet process, the BNP posterior of entropy can be proposed as follows. Assume that \( x_{d \times n} = (x_1, \ldots, x_n) \) is an observed sample of size \( n \) from an unknown \( d \)-variate distribution \( F \), where \( x_i \in \mathbb{R}^d \), \( i = 1, \ldots, n \). Note that, the subscript \( d \times n \) may be omitted whenever it is clear in the context. To present the BNP posterior of entropy, we use the prior \( F \sim DP(a,G) \) for some choices of \( a \) and \( d \)-variate distribution \( G \). By (5), \( F^* := F|x \sim DP(a + n, G_{a,n}^*). \) The BNP posterior of entropy is
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proposed by

\[ H_{N,a+n,k}^{pos} = \sum_{i=1}^{N} J_{i,N}^{*} \left( \log \left( \frac{(N-1)\pi^{d/2}}{k\Gamma \left( \frac{d}{2} + 1 \right)} \right) - L_{k-1} + \gamma + \log k \right), \]

(12)

where \((J_{i,N}^{*})_{1 \leq i \leq N} \sim \text{Dirichlet}((a+n)/N, \ldots, (a+n)/N)\), \(Y_1^*, \ldots, Y_N^* \sim G_{a,n}^*\) and

\[ k \in \{1, \ldots, N-1\}. \]

In the same manner, for \(i = 1, \ldots, d\), the marginal entropy \(H(F_i)\) can be estimated by using prior \(F_i \sim DP(a, G_i)\), where \(G_i\) is the \(i\)-th marginal of the cdf \(G\). The convergence of \(E(H_{N,a+n,k}^{pos})\) to the entropy of the true distribution will be shown in the next theorem. As we will show later, the entropy of \(G_{a,n}^*\) has a crucial role in the proof of this convergence. To carry on, some notations and theoretical results related to \(H(G_{a,n}^*)\) are first presented.

Let \(F_1, \ldots, F_m\) be \(m\) cdf’s defined on the same probability space and \(F_{\alpha} = \sum_{i=1}^{m} \alpha_i F_i\) so that \(\sum_{i=1}^{m} \alpha_i = 1\). The following result due to Toomaj and Zarei (2017, p. 4226) gives the entropy of \(F_{\alpha}\). Let \(D_{kull}(F_i, F_{\alpha})\) denote the Kullback-Leibler divergence between \(F_i\) and \(F_{\alpha}, i = 1, \ldots, m\), then

\[ H(F_{\alpha}) = \sum_{i=1}^{m} \alpha_i H(F_i) + \sum_{i=1}^{m} \alpha_i D_{kull}(F_i, F_{\alpha}). \]

(13)

Now, by applying (13) for (5), we have

\[ H(G_{a,n}^*) = \frac{a}{a+n} H(G) + \frac{n}{a+n} H(F_n) + \frac{n}{a+n} D_{kull}(F_n, G_{a,n}^*) + \frac{a}{a+n} D_{kull}(G, G_{a,n}^*). \]

(14)

Note that, \(D_{kull}(\cdot, \cdot)\) is only defined for two cdf’s on the same probability space (both cdf’s should be continuous or discrete). Since \(G_{a,n}^*\) is not completely continuous or discrete, \(D_{kull}(G, G_{a,n}^*)\) and \(D_{kull}(F_n, G_{a,n}^*)\) in (14) do not make sense. To avoid this difficulty, we define \(D_{kull}(G, G_{a,n}^*)\) and \(D_{kull}(F_n, G_{a,n}^*)\) by encoding the distributions \(G, F_n\) and \(G_{a,n}^*\) around a set of the \(d\)-dimensional real valued points through the next lemma. In fact, we use a method of discretization to define \(G, F_n\) and \(G_{a,n}^*\) on a same probability space.

Lemma 3 Consider \(G, F_n\) and \(G_{a,n}^*\) as defined in (5). Let \(I \subseteq \mathbb{N}\) and \(\{t_j\}_{j \in I} \subseteq \mathbb{R}^d\) be
such that for a given \( \delta > 0 \)

\[
g_j = \Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, \ldots, t_{jd} - \delta < Z_d \leq t_{jd})
= G(t_{j1}, \ldots, t_{jd}) + (2^d - 3)G(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_{S} G(s_1, \ldots, s_d), \tag{15}
\]

\[
f_{j,n} = \Pr(t_{j1} - \delta < Z'_1 \leq t_{j1}, \ldots, t_{jd} - \delta < Z'_d \leq t_{jd})
= F_n(t_{j1}, \ldots, t_{jd}) + (2^d - 3)F_n(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_{S} F_n(s_1, \ldots, s_d), \tag{16}
\]

and

\[
g_{j,a,n} = \Pr(t_{j1} - \delta < Z''_1 \leq t_{j1}, \ldots, t_{jd} - \delta < Z''_d \leq t_{jd})
= G_{a,n}(t_{j1}, \ldots, t_{jd}) + (2^d - 3)G_{a,n}(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_{S_d} G_{a,n}(s_1, \ldots, s_d). \tag{17}
\]

satisfy conditions \( g_j = 0 \) and \( f_{j,n} = 0 \) whenever \( g_{j,a,n} = 0 \), \( \sum_{j \in I} g_{j,a,n} \leq \sum_{j \in I} g_j \leq 1 \), \( \sum_{j \in I} f_{j,n} \leq 1 \), where \( Z \sim G \), \( Z' \sim F_n \), \( Z'' \sim G_{a,n} \) and \( S_d = \{(s_1, \ldots, s_d) : s_k \in \{t_{jk} - \delta, t_{jk}\}, k \in \{1 \ldots d\}\} \setminus \{(t_{j1}, \ldots, t_{jd}), (t_{j1} - \delta, \ldots, t_{jd} - \delta)\} \). \( D_{\text{kull}}(G, G_{a,n}) \) and \( D_{\text{kull}}(F_n, G_{a,n}) \), respectively, can be (empirically) defined as \( \sum_{j \in I} (g_j \log \frac{g_j}{g_{j,a,n}}) \) and \( \sum_{j \in I} (f_{j,n} \log \frac{f_{j,n}}{g_{j,a,n}}) \) by applying the general definition of the Kullback-Leibler (MacKay, 2003, p. 34) based on atoms \( g_j, f_{j,n} \) and \( g_{j,a,n} \) with the standard convention \( 0 \log \frac{0}{0} = 0 \) (Piera and Parada, 2009, p. 91).

Proof. An inductive procedure to derive (15), (16) and (17) is given by Appendix A. ■

Note that defining \( g_j, f_{j,n} \) and \( g_{j,a,n} \), respectively, based on \( G \), \( F_n \) and \( G_{a,n} \) play a key role in the proof of the next theorem.

Theorem 4 Let \( x_{d \times n} \) be a sample from \( d \)-variate distribution function \( F \) and \( F|x \sim DP(a + n, G_{a,n}) \). Assume that the limit of \( D_{\text{kull}}(G, G_{a,n}) \) exists, as \( n \to \infty \). Then, \( E(H_{N,a+n,k}^{\text{pos}}) \to H(F) \), as \( N \to \infty \) and \( n \to \infty \).

Proof. From the conjugacy property of the Dirichlet process, part (i) of Lemma (1) implies that \( E(H_{N,a+n,k}^{\text{pos}}) \to H(G_{a,n}) \), as \( N \to \infty \). Consider \( H(G_{a,n}) \) as defined in (14).
Then, \( \frac{a}{a+n} H(G) \to 0 \) as \( n \to \infty \). Also, the strong law of large numbers implies that \( H(F_n) = -n^{-1} \sum_{i=1}^{n} \log(f(x_i)) \to H(F) \) as \( n \to \infty \). Now, consider \( D_{\text{kull}}(F_n, G_{a,n}^*) \) as given by Lemma 3. From (5) and (17), we get

\[
g_{j,a,n}^* = \frac{a}{a+n} G(t_{j1}, \ldots, t_{jd}) + \frac{n}{a+n} F_n(t_{j1}, \ldots, t_{jd}) + (2^d - 3) \left\{ \frac{a}{a+n} G(t_{j1} - \delta, \ldots, t_{jd} - \delta) \ight. \\
\left. + \frac{n}{a+n} F_n(t_{j1} - \delta, \ldots, t_{jd} - \delta) \right\} - \sum_S \left( \frac{a}{a+n} G(s_1, \ldots, s_d) + \frac{n}{a+n} F_n(s_1, \ldots, s_d) \right).
\]

After some simplification, we have

\[
g_{j,a,n}^* = \frac{a}{a+n} \left\{ G(t_{j1}, \ldots, t_{jd}) + (2^d - 3)G(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_S G(s_1, \ldots, s_d) \right\} \\
+ \frac{n}{a+n} \left\{ F_n(t_{j1}, \ldots, t_{jd}) + (2^d - 3)F_n(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_S F_n(s_1, \ldots, s_d) \right\}.
\]

Now, using (15) and (16), we have \( g_{j,a,n}^* = \frac{a}{a+n} g_j + \frac{n}{a+n} f_{j,n} \). Clearly, \( g_{j,a,n}^* \geq \frac{n}{a+n} f_{j,n} \), which concludes that \( \frac{f_{j,n}}{g_{j,a,n}^*} \leq 1 + a/n \leq 1 + a \), for \( j \in I \). Consequently, \( D_{\text{kull}}(F_n, G_{a,n}^*) \leq \log(1 + a) < \infty \). On the other hand, applying the Glivenko-Cantelli theorem in (16) and (17) implies \( f_{j,n} \xrightarrow{a.s.} f_j \) and \( g_{j,a,n}^* \xrightarrow{a.s.} g_j \), as \( n \to \infty \), where \( f_j \) denotes \( F(t_{j1}, \ldots, t_{jd}) + F(t_{j1} - \delta, \ldots, t_{jd} - \delta) - \sum_S F(s_1, \ldots, s_d) \). Hence, by the discrete version of the dominated convergence theorem, we have

\[
D_{\text{kull}}(F_n, G_{a,n}^*) = \sum_{j \in I} f_{j,n}(\log f_{j,n} - \log g_{j,a,n}^*) \xrightarrow{a.s.} \sum_{j \in I} f_j(\log f_j - \log f_j) = 0.
\]

The proof is completed by letting \( n \to \infty \) in the last term of (14).

### 3.2 Posterior of Mutual Information

The proposed BNP posterior of mutual information takes the form:

\[
MI_{\text{pos}} = \left[ -H_{N,a+n,k}^{\text{pos}}(F) + \sum_{i=1}^{d} H_{N,a+n,k}^{\text{pos}}(F_i) \right]^+,
\]

where \( b^+ = \max(b, 0) \). Note that, the proposed estimator ensures the non-negativity of the BNP mutual information estimation. The BNP test in the next section will be proposed based on \( MI_{\text{pos}} \). Since implementation of \( MI_{\text{pos}} \) requires considering choices of
a and $G$ in $H_{N,a+n,k}^{\text{pos}}$. Hence, it is necessary to look carefully at the impact of these two ingredients on the approach. For instance, $G$ should be chosen to ensure compatibility between $G$ and data. That is, to avoid the so-called “prior-data conflict” (Evans and Moshonov, 2006). As for $a$, we assess the effect of this parameter on $H_{N,a+n,k}^{\text{pos}}$ for fixed $n$ as $N \to \infty$ in the next theorem.

**Theorem 5** Let $x_{d \times n}$ be a sample from $d$-variate distribution function $F$ and $F|\mathbf{x} \sim \text{DP}(a+n,G_{a,n}^*)$. Then, for a fixed $n$, $\lim \inf E(H_{N,a+n,k}^{\text{pos}}) \geq H(F) + c$ as $N \to \infty$ and $a \to \infty$, where $c \neq 0$.

**Proof.** For fixed $a$ and $n$, similar to the proof of Theorem 4, $E(H_{N,a+n,k}^{\text{pos}}) \to H(G_{a,n}^*)$, as $N \to \infty$. Now, since $D_{\text{kul}}(G,G_{a,n}^*)$ and $D_{\text{kul}}(F_n,G_{a,n}^*)$ are non-negative in (14), we have $H(G_{a,n}^*) \geq \frac{a}{a+n} H(G) + \frac{n}{a+n} H(F_n) = I_1 + I_2$. Letting $a \to \infty$ in $I_1$ and $I_2$ gives

$$\lim \inf H(G_{a,n}^*) \geq H(G) = (H(G) - H(F)) + H(F) = c + H(F).$$

Since the prior guess $G$ is not the same as the true distribution $F$, then $c \neq 0$ and the proof is completed. ■

### 4 Prior-based Test for Independence

Let $\mathbf{X} = (X_1, \ldots, X_d)$ be a random vector from an unknown distribution $F$. The problem to be addressed in this section is assessing the hypothesis

$$\mathcal{H}_0 : MI(F) = 0,$$

using BNP framework. Let $x_{d \times n}$ be an observed sample of size $n$ from $F \sim \text{DP}(a,G)$. In order to implement the test, for a given choice of $a$, let $G$ be the cdf of $N(0_d, I_d)$ and $MI^{\text{pri}} = [-H_{N,a,k}^{\text{pri}}(F) + \sum_{i=1}^d H_{N,a,k}^{\text{pri}}(F_i)]^+$ be the prior of mutual information between elements of $\mathbf{X}$. From part (i) of Lemma 1, since $E(MI^{\text{pri}}) \to MI(G) = 0$ as $N \to \infty$, then $MI^{\text{pri}}$ is a good prior to compare with $MI^{\text{pos}}$ for displaying the mutual independence between $X_1, \ldots, X_d$. As shown in Theorem 4, if the assumption of independence
A test for independence via BNP estimation of MI

is true, the distribution of $MI^{pos}$ (posterior of mutual information) should be more concentrated around zero than the distribution of $MI^{pri}$ (i.e. $MI^{pos}$ more supports $H_0$ than $MI^{pri}$); otherwise, the distribution of $MI^{pri}$ should be more concentrated at zero than the distribution of $MI^{pos}$ (i.e. $MI^{pri}$ more supports $H_0$ than $MI^{pos}$). This comparison is made by using RB with the interpretation as discussed in Section 2. To this end, we consider an interval $[0, c)$ to compare the concentration of the distribution of the posterior to the prior. The choice of $c$ has a key role in the proposed test. As a simple tactic, we propose to fix $c$ to be close to zero (such as $c = 0.05$) such that the prior probability $Pr(MI^{pri} \in [0, c)) = 0.5$. Note that, the value of $Pr(MI^{pri} \in [0, c))$ depends on the choice of the concentration parameter $a$ in $DP(a, G)$. As Lemma 1 shows, for small values of $a$, the concentration of $MI^{pri}$ will be decreased around zero. Then, the errors of $MI^{pri}$ (i.e. large values of $MI^{pri}$) will be increased. This may cause to decrease the value of $Pr(MI^{pri} \in [0, c))$, which may lead to have incorrect values for RB. To avoid this difficulty, we need to increase the value of $a$ such that $a$ does not exceed $n/2$. Hence, contrary to the estimation problem where $a$ should be selected to be small, the choice of $a$ in the test is different. Algorithm A helps to elicit suitable choices for $a$ to run the test.

**Algorithm A: Selecting $a$ in $MI^{pri}$ for testing of independence**

i. Set a small fixed value $c$, say $c = 0.05$.

ii. Choose the value of $a$ such that $Pr(0 \leq MI^{pri} < c) = 0.5$. The preceding probability can be estimated as follows:

a. Generate a sample of $r$ values from $MI^{pri}$. The steps of sampling from $MI^{pri}$ are detailed in Algorithms B, Section 5.

b. Consider the ratio of the values of $MI^{pri}$ contents of $[0, c)$ as the approximation of $Pr(0 \leq MI^{pri} < c)$.

c. If the approximated probability is more (less) than 0.5, then decrease (increase) the value of $a$ to reach the value of 0.5.

Algorithm A was thoroughly implemented for several values of $c$ and $d$. Table 4 in Appendix B reports appropriate values of $a$ when $d = 2$. The results for $d > 2$ are found
to be similar. That is, Table 4 may be used for any arbitrary dimension \(d\). Thus, from Table 4, an appropriate choice of \(a\) to carry out the test is \(a = 1\).

5 Computational Algorithms for Testing of Independence

The following algorithms summarize the main steps to carry out the test of independence for (18). Since closed forms of densities of \(\text{MI}^{\text{pri}}\) and \(\text{MI}^{\text{pos}}\) are not available, their empirical distributions are required to implement the below algorithms.

**Algorithm B: Prior-based test for independence**

1. Use Algorithm A to choose a value of \(a\). Note that, \(a = 1\) is a recommended choice to proceed the test.
2. For the selected \(a\) in the previous step, let \(G\) be the cdf of \(N(0_d, I_d)\) and generate a sample from \(DP(a, G)\) as described in Section 2.1.
3. For the sample generated in the previous step, use (9) to compute \(H_{N,a,k}^{\text{pri}}(F)\) and \(H_{N,a,k}^{\text{pri}}(F_i)\), for \(i = 1, \ldots, d\).
4. Substitute \(H_{N,a,k}^{\text{pri}}(F)\) and \(H_{N,a,k}^{\text{pri}}(F_i)\)'s into (2) to compute \(\text{MI}^{\text{pri}} = [-H_{N,a,k}^{\text{pri}}(F) + \sum_{i=1}^{d} H_{N,a,k}^{\text{pri}}(F_i)]^+\).
5. Repeat steps 2-4 to generate a sample of \(\ell\) values from \(\text{MI}^{\text{pri}}\).
6. Use steps 2-5 to obtain a sample of \(\ell\) values from \(\text{MI}^{\text{pos}}\) by replacing \(a\) by \(a + n\), \(G\) by \(G^*_{a,n}\), (9) by (12) and prior by posterior.
7. Let \(\hat{F}_{\text{MI}^{\text{pri}}}\) denote the empirical cdf of \(\text{MI}^{\text{pri}}\) based on the prior sample in step (2). Let \(\hat{F}_{\text{MI}^{\text{pos}}}\) denote the empirical cdf of \(\text{MI}^{\text{pos}}\) based on the posterior sample in step (3). Estimate \(\overline{\text{RB}}_{\text{MI}}(0|\mathbf{x}) = \pi_{\text{MI}^{\text{pos}}}(0)/\pi_{\text{MI}^{\text{pri}}}(0)\) by

\[
\overline{\text{RB}}_{\text{MI}}(0|\mathbf{x}) = \left\{\hat{F}_{\text{MI}^{\text{pos}}}(c) - \hat{F}_{\text{MI}^{\text{pos}}}(0)\right\}/\left\{\hat{F}_{\text{MI}^{\text{pri}}}(c) - \hat{F}_{\text{MI}^{\text{pri}}}(0)\right\},
\]

(19)

8. Let \(M\) be a positive number. For \(i = 0, \ldots, M\), let \(\hat{d}_{i/M}\) be the estimate of \(d_{i/M}\), the \((i/M)\)-th prior quantile of \(\text{MI}^{\text{pri}}\). Here \(\hat{d}_0\) and \(\hat{d}_1\) are, respectively, the smallest and the
largest value of the $r$ values generated in step (2). For $d \in (\hat{d}_0, \hat{d}_1)$, estimate the strength $DP_{MI}(RB_{MI}(d \mid x) \leq RB_{MI}(0 \mid x) \mid x)$ by the finite sum

$$
\sum_{i \geq i_0} (\hat{F}_{MI}^{ pos}(\hat{d}_{i/M}) - \hat{F}_{MI}^{ pos}(\hat{d}_{i/M})),
$$

(20)

where $i_0$ is chosen so that $\frac{i_0}{M}$ is not too small (typically $\frac{i_0}{M} \approx 0.05$) and $\hat{R}B_{MI}(\hat{d}_{i/M} \mid x) = M\{\hat{F}_{MI}^{ pos}(\hat{d}_{(i+1)/M}) - \hat{F}_{MI}^{ pos}(\hat{d}_{i/M})\}$. For fixed $M$, as $N \to \infty$ and $\ell \to \infty$, then $\hat{d}_{i/M}$ converges almost surely to $d_{i/M}$ and (19) and (20) converge almost surely to $RB_{MI}(0 \mid x)$ and $DP_{MI}(RB_{MI}(d \mid x) \leq RB_{MI}(0 \mid x) \mid x)$, respectively. The consistency of the proposed test is achieved by Proposition 6 of Al-Labadi and Evans (2018).

6 Simulation Studies

This section reveals the performance of the BNP methodology in testing of independence. To this aim, samples are generated from several $d$-variate distributions. Table 5 gives the relevant notations of these distributions. First, we consider three common $d$-variate distributions: normal, $t$-student and Maxwell-Boltzmann distributions. We consider sample sizes $n = 20, 30$ and 50. For each sample size, $r = 1000$ samples were generated. Each sample gives an $RB$ (strength) by setting $k = 3$ in Algorithm B. For the test, we set $\ell = 1000$ in Algorithm B. With regard to Table 4, we set $c = 0.05$ and thus choose $a = 1$ as outlined in Table 4. The recorded values of $RB$ and strength (Str) are the average of the 1000 results. For the goal of comparison, the p-value of the test of independence (Berrett and Samworth, 2019b) are reported in $r$ replication. The R package IndepTest is used to compute the p-value. The results of the BNP method and its frequentist counterpart (Berrett et al., 2019a; Berrett and Samworth, 2019b) are presented in Table 1. It follows from Table 1 that the prior based test has a good performance to test independence between $d$ variables. To clear up, for instance, when $N_4(0_4, \Sigma_4)$ and $n = 50$ in Table 1, the average value of relative belief ratios is 0.53 with relevant strength 0.07, which shows the good performance of the proposed test to reject the assumption of mutual independence.
Table 1: The average values of RB(strength) for testing the mutually independent under several distributions with $k = 3$.

| Example       | $d$ (MFr) | n  | BNP  | Berrett et al. |
|---------------|-----------|----|------|----------------|
|               |           |    | RB(St)* | p-value        |
| $N_{d}(0, I_d)$ | 2         | 20 | 1.97(0.53) | 0.498          |
|               | (0.066)   | 30 | 2.08(0.48) | 0.508          |
|               |           | 50 | 2.11(0.52) | 0.493          |
|               | 3         | 20 | 1.99(0.56) | 0.514          |
|               | (0.110)   | 30 | 2.15(0.58) | 0.507          |
|               |           | 50 | 2.38(0.57) | 0.494          |
|               | 4         | 20 | 2.02(0.62) | 0.509          |
|               | (0.195)   | 30 | 2.32(0.56) | 0.505          |
|               |           | 50 | 2.49(0.63) | 0.508          |
| $N_{d}(0, \Sigma_d)$ | 2         | 20 | 1.59(0.37) | 0.401          |
|               | (0.066)   | 30 | 1.53(0.34) | 0.366          |
|               |           | 50 | 1.45(0.21) | 0.348          |
|               | 3         | 20 | 1.06(0.12) | 0.269          |
|               | (0.235)   | 30 | 0.91(0.09) | 0.228          |
|               |           | 50 | 0.78(0.05) | 0.164          |
|               | 4         | 20 | 0.98(0.13) | 0.230          |
|               | (0.450)   | 30 | 0.72(0.09) | 0.160          |
|               |           | 50 | 0.51(0.05) | 0.109          |
| $N_{d}(0, A_d)$ | 2         | 20 | 0.91(0.09) | 0.297          |
|               | (0.143)   | 30 | 0.63(0.06) | 0.267          |
|               |           | 50 | 0.56(0.04) | 0.214          |
|               | 3         | 20 | 1.27(0.21) | 0.312          |
|               | (0.143)   | 30 | 1.06(0.10) | 0.265          |
|               |           | 50 | 0.64(0.09) | 0.198          |
|               | 4         | 20 | 1.85(0.31) | 0.317          |
|               | (0.143)   | 30 | 1.71(0.39) | 0.275          |
|               |           | 50 | 0.91(0.18) | 0.220          |
Similar to the study of Roy et al. (2019), to consider more interesting scenarios, we included the following six unusual bivariate distributions (UBD):

**Four clouds:** Let \( Z_1, Z_2, T_1 \) and \( T_2 \) be independent with \( Z_1, Z_2 \sim N_1(0,1) \) and \( \Pr(T_1 = \pm 1) = \Pr(T_2 = \pm 1) = \frac{1}{2} \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = Z_1 + T_1 \) and \( X_2 = Z_2 + T_2 \).

**Circle:** Let \( Z_1, Z_2 \) and \( U \) be independent with \( Z_1, Z_2 \sim N_1(0,1) \) and \( U \sim U(-1,1) \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = \sin(\pi U) + Z_1/8 \) and \( X_2 = \cos(\pi U) + Z_2/8 \).

**Two Parabolas:** Let \( U_1, U_2 \) and \( T \) be independent with \( U_1 \sim U(-1,1), U_2 \sim U(0,1) \) and \( \Pr(T = \pm 1) = 1/2 \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = U_1 \) and \( X_2 = T(U_1^2 + U_2^2)/2 \).

**Parabola:** Let \( U_1 \) and \( U_2 \) be independent with \( U_1 \sim U(-1,1) \) and \( U_2 \sim U(0,1) \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = U_1 \) and \( X_2 = (U_1^2 + U_2^2)/2 \).

**Diamond:** Let \( U_1, U_2 \overset{i.i.d.}{\sim} U(-1,1) \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = U_1 \cos(-\pi/4) + U_2 \sin(-\pi/4) \) and \( X_2 = -U_1 \sin(-\pi/4) + U_2 \cos(-\pi/4) \).

**W:** Let \( U_1 \) and \( U_2 \) be independent with \( U_1 \sim U(-1,1) \) and \( U_2 \sim U(0,1) \). Then, consider the random vector \((X_1, X_2)\) with \( X_1 = U_1 + U_2/3 \) and \( X_2 = 4((U_1^2 - 1/2)^2 + U_2/n) \).

Figure 1 shows plots of samples generated from the above distributions. The interesting property of these distributions is that in each pair of random variables, \( X_1 \) and \( X_2 \) are uncorrelated but dependent, except in four clouds where \( X_1 \) and \( X_2 \) are uncorrelated and independent. Table 2 shows that the assumption of mutual independence is accepted only for four clouds in the cases where the sample size is greater than or equal to 30.

Finally, to evaluate the performance of the proposed method on a real data set, the combined cycle power plant (CCPP) data set is considered. This data set contains 9568 five-dimensional data points. It is collected from 2006 to 2011 and is available at https://archive.ics.uci.edu/ml/datasets/combined+cycle+power+plant. Its goal is to predict the net hourly electrical energy output of the plant based on the temperature (T), the ambient pressure (AP), the relative humidity (RH) and the exhaust vacuum (V). Thus, it is significant to check whether the four variables T, AP, RH, and V are independent. In addition, besides using all 9568 data points, we considered three samples with
Figure 1: Samples generated from six UBDs with sample size of $n = 100$.

sample sizes $n = 20, 30$ and $50$ generated randomly from the whole data set. The proposed method then is implemented. The results are reported in Table 3, where it follows clearly from this table that the assumption of independence between T, AP, RH and V is rejected in all cases.

7 Concluding Remarks

The BNP prior and posterior of mutual information have been proposed. They have been constructed based on using the Dirichlet process and the $k$-nearest neighbor distance. Several interesting theoretical results have been presented. As a result, a new Bayesian test of independence has been developed. The performance of the procedure has been examined by several interesting examples. The obtained results reflect the excellent performance of the methodology in testing.
Table 2: The average values of the RB and its Str over r samples generated from six UBDs with k = 3.

| UBD            | RB  | Str | p-value | UBD            | RB  | Str | p-value |
|----------------|-----|-----|---------|----------------|-----|-----|---------|
| Four clouds    | 20  | 1.67| 0.40    | 0.493          | Parabola       | 20  | 0.88| 0.26    | 0.061          |
|                | 30  | 2.17| 0.48    | 0.498          | 30  | 0.66| 0.12    | 0.036          |
|                | 50  | 2.25| 0.57    | 0.499          | 50  | 0.46| 0.09    | 0.009          |
| Circle         | 20  | 0.97| 0.21    | 0.178          | Diamond        | 20  | 1.07| 0.23    | 0.346          |
|                | 30  | 0.60| 0.08    | 0.049          | 30  | 0.89| 0.20    | 0.273          |
|                | 50  | 0.19| 0.00    | 0.009          | 50  | 0.77| 0.12    | 0.175          |
| Two parabolas  | 20  | 0.74| 0.15    | 0.045          | W             | 20  | 1.71| 0.49    | 0.174          |
|                | 30  | 0.31| 0.03    | 0.012          | 30  | 0.99| 0.22    | 0.064          |
|                | 50  | 0.13| 0.01    | 0.009          | 50  | 0.62| 0.02    | 0.009          |

Table 3: The result of the BNP test (RB and strength) and the p-value of the test of Berrett and Samworth (2019b) for CCPP data set with k = 3 and various sample sizes n.

| CCPP n | RB(Str) | p-value |
|--------|---------|---------|
| 20     | 0.65(0.07) | 0.237   |
| 30     | 0.60(0.02) | 0.019   |
| 50     | 0.29(0.01) | 0.009   |
| 9568   | 0.10(0.00) | 0.009   |

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Appendix A  Proof of Equation (15), (16) and (17)

We show (15) by two below steps (the proof for (16) and (17) are similar).

Step 1: For $d = 3$, consider $Z = (Z_1, Z_2, Z_3) \sim G$ and $\{t_j\}_{j \in I} \subseteq \mathbb{R}^3$, where $t_j = (t_{j1}, t_{j2}, t_{j3})$. Then for a given $\delta > 0$, we can write

$$
Pr(Z_1 \leq t_{j1}, Z_2 \leq t_{j2}, Z_3 \leq t_{j3}) = Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, t_{j2} - \delta < Z_2 \leq t_{j2}, t_{j3} - \delta < Z_3 \leq t_{j3})
$$

$$
+ Pr(Z_1 \leq t_{j1} - \delta, t_{j2} - \delta < Z_2 \leq t_{j2}, t_{j3} - \delta < Z_3 \leq t_{j3})
$$

$$
+ Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, Z_2 \leq t_{j2} - \delta, t_{j3} - \delta < Z_3 \leq t_{j3})
$$

$$
+ Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, t_{j2} - \delta < Z_2 \leq t_{j2}, Z_3 \leq t_{j3} - \delta)
$$

$$
+ Pr(Z_1 \leq t_{j1} - \delta, Z_2 \leq t_{j2} - \delta, t_{j3} - \delta < Z_3 \leq t_{j3})
$$

$$
+ Pr(Z_1 \leq t_{j1} - \delta, t_{j2} - \delta < Z_2 \leq t_{j2}, Z_3 \leq t_{j3} - \delta)
$$

$$
+ Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, Z_2 \leq t_{j2} - \delta, Z_3 \leq t_{j3} - \delta)
$$

$$
+ Pr(Z_1 \leq t_{j1} - \delta, Z_2 \leq t_{j2} - \delta, Z_3 \leq t_{j3} - \delta)
$$

$$
= I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7 + I_8.
$$

(21)

On the other hand,

$$
I_2 + Pr(Z_1 \leq t_{j1} - \delta, Z_2 \leq t_{j2} - \delta, Z_3 \leq t_{j3} - \delta) = Pr(Z_1 \leq t_{j1} - \delta, Z_2 \leq t_{j2}, Z_3 \leq t_{j3}).
$$

Then, we have

$$
I_2 = G(t_{j1} - \delta, t_{j2}, t_{j3}) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta).
$$

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Similarly,

\[ I_3 = G(t_{j1}, t_{j2} - \delta, t_{j3}) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta), \]
\[ (23) \]

\[ I_4 = G(t_{j1}, t_{j2}, t_{j3} - \delta) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta), \]
\[ (24) \]

\[ I_5 = G(t_{j1} - \delta, t_{j2} - \delta, t_{j3}) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta), \]
\[ (25) \]

\[ I_6 = G(t_{j1} - \delta, t_{j2}, t_{j3} - \delta) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta), \]
\[ (26) \]

\[ I_7 = G(t_{j1}, t_{j2} - \delta, t_{j3} - \delta) - G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta). \]
\[ (27) \]

by substituting (22), (23), (24), (25), (26), and (27) into (21), we have

\[ G(t_{j1}, t_{j2}, t_{j3}) = Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, t_{j2} - \delta < Z_2 \leq t_{j2}, t_{j3} - \delta < Z_3 \leq t_{j3}) \]
\[ + G(t_{j1} - \delta, t_{j2}, t_{j3}) + G(t_{j1}, t_{j2} - \delta, t_{j3}) + G(t_{j1}, t_{j2}, t_{j3} - \delta) \]
\[ + G(t_{j1} - \delta, t_{j2} - \delta, t_{j3}) + G(t_{j1} - \delta, t_{j2}, t_{j3} - \delta) + G(t_{j1}, t_{j2} - \delta, t_{j3} - \delta) \]
\[ + (-2^3 - 2 + 1) G(t_{j1}, t_{j2}, t_{j3}). \]

After simplification, we get

\[ Pr(t_{j1} - \delta < Z_1 \leq t_{j1}, t_{j2} - \delta < Z_2 \leq t_{j2}, t_{j3} - \delta < Z_3 \leq t_{j3}) = G(t_{j1}, t_{j2}, t_{j3}) \]
\[ + (2^3 - 3) G(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta) \]
\[ - \sum_{s_3} G(s_1, s_2, s_3), \]

where \( S_3 = \{(s_1, s_2, s_3) : s_k \in \{t_{jk} - \delta, t_{jk}\}, k \in \{1, 2, 3\} \} \setminus \{(t_{j1} - \delta, t_{j2} - \delta, t_{j3} - \delta), (t_{j1}, t_{j2}, t_{j3})\}. \)

Step 2: Now, generalize step 1 for \( d > 3 \) to conclude the result.
Appendix B

Table 4: Values of $Pr(MI^{pri} \in [0, c))$ in Algorithm A to choose $c$ for the BNP test of independence with $k = 3$ and $d = 2$.

| $c$  | $a = 0.05$ | $a = 1$ | $a = 5$ | $a = 10$ |
|------|------------|---------|---------|---------|
| 0.01 | 0.314      | 0.473   | 0.477   | 0.490   |
| 0.02 | 0.317      | 0.479   | 0.486   | 0.499   |
| 0.03 | 0.323      | 0.481   | 0.495   | 0.510   |
| 0.04 | 0.325      | 0.491   | 0.510   | 0.520   |
| 0.05 | 0.327      | 0.498   | 0.521   | 0.538   |
| 0.06 | 0.331      | 0.516   | 0.533   | 0.549   |
| 0.07 | 0.333      | 0.520   | 0.549   | 0.563   |
| 0.08 | 0.337      | 0.533   | 0.554   | 0.579   |
| 0.09 | 0.342      | 0.548   | 0.576   | 0.601   |
| 0.1  | 0.344      | 0.568   | 0.600   | 0.626   |

Table 5: Description of notations

1. $c_2 := (c, c)^T$, $I_2 := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $A_2 := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$, $A_3 := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$, $\Sigma_4 := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$.

2. $U(a, b)$: A univariate uniform distribution with parameters $a$ and $b$.

3. $F_1 \otimes \ldots \otimes F_d$: A $d$-variate distribution with $d$ independent marginal distributions $F_1, \ldots, F_d$.

4. $Mwell(c_d) = Mwell(c) \otimes \ldots \otimes Mwell(c)$ denotes the Maxwell-Boltzman distribution with scale parameter $c$ and $MI^T = 0.5$.

5. $N_d(0_d, \Sigma_d)$: A $d$-variate normal distribution with mean vector $0_d$ and covariance matrix $\Sigma_d$, and $MI^T = \frac{d}{2} \log((2\pi e)^d \det(\Sigma)) - \frac{1}{2} \log((2\pi e)^d \det(\Sigma))$, where $\sigma^2_d$ is the $i$-th diagonal element of $\Sigma_d$.

6. $t_r(0_d, I_d)$: A $d$-variate $t$-student distribution with location parameter $0_d$, scale parameter $I_d$ and $r$ degrees of freedom, and $MI^T = \frac{d}{2} \log((2\pi e)^d \det(\Sigma)) - \frac{1}{2} \log((2\pi e)^d \det(\Sigma))$, where $\sigma^2_d$ is the $i$-th diagonal element of $\Sigma_d$.

7. $SP_d(LN(0, 0.25))$: A $d$-variate spherical distribution with lognormal distribution $LN(0, 0.25)$ for radii.

† Required R packages: shotGroups and distrEllipse.