Nonparametric independence testing via mutual information

Thomas B. Berrett and Richard J. Samworth
Statistical Laboratory, University of Cambridge
November 20, 2017

Abstract

We propose a test of independence of two multivariate random vectors, given a sample from the underlying population. Our approach, which we call MINT, is based on the estimation of mutual information, whose decomposition into joint and marginal entropies facilitates the use of recently-developed efficient entropy estimators derived from nearest neighbour distances. The proposed critical values, which may be obtained from simulation (in the case where one marginal is known) or resampling, guarantee that the test has nominal size, and we provide local power analyses, uniformly over classes of densities whose mutual information satisfies a lower bound. Our ideas may be extended to provide a new goodness-of-fit tests of normal linear models based on assessing the independence of our vector of covariates and an appropriately-defined notion of an error vector. The theory is supported by numerical studies on both simulated and real data.

1 Introduction

Independence is a fundamental concept in statistics and many related fields, underpinning the way practitioners frequently think about model building, as well as much of statistical theory. Often we would like to assess whether or not the assumption of independence is reasonable, for instance as a method of exploratory data analysis (Steuer et al., 2002; Albert et al., 2015; Nguyen and Eisenstein, 2017), or as a way of evaluating the goodness-of-fit of a statistical model (Einmahl and van Keilegom, 2008). Testing independence and estimating dependence
are well-established areas of statistics, with the related idea of the correlation between two random variables dating back to Francis Galton’s work at the end of the 19th century (Stigler, 1989), which was subsequently expanded upon by Karl Pearson (e.g. Pearson, 1920). Since then many new measures of dependence have been developed and studied, each with its own advantages and disadvantages, and there is no universally accepted measure. For surveys of several measures, see, for example, Schweizer (1981), Joe (1989), Mari and Kotz (2001) and the references therein. We give an overview of more recently-introduced quantities below; see also Josse and Holmes (2016).

In addition to the applications mentioned above, dependence measures play an important role in independent component analysis (ICA), a special case of blind source separation, in which a linear transformation of the data is sought so that the transformed data is maximally independent; see e.g. Comon (1994), Bach and Jordan (2002), Miller and Fisher (2003) and Samworth and Yuan (2012). Here, independence tests may be carried out to check the convergence of an ICA algorithm and to validate the results (e.g. Wu, Yu and Li, 2009). Further examples include feature selection, where one seeks a set of features which contains the maximum possible information about a response (Torkkola, 2003; Song et al., 2012), and the evaluation of the quality of a clustering in cluster analysis (Vinh, Epps and Bailey, 2010).

When dealing with discrete data, often presented in a contingency table, the independence testing problem is typically reduced to testing the equality of two discrete distributions via a chi-squared test. Here we will focus on the case of distributions that are absolutely continuous with respect to the relevant Lebesgue measure. Classical nonparametric approaches to measuring dependence and independence testing in such cases include Pearson’s correlation coefficient, Kendall’s tau and Spearman’s rank correlation coefficient. Though these approaches are widely used, they suffer from a lack of power against many alternatives; indeed Pearson’s correlation only measures linear relationships between variables, while Kendall’s tau and Spearman’s rank correlation coefficient measure monotonic relationships. Thus, for example, if \(X\) has a symmetric distribution on the real line, and \(Y = X^2\), then the population quantities corresponding to these test statistics are zero in all three cases. Hoeffding’s test of independence (Hoeffding, 1948) is able to detect a wider class of departures from independence and is distribution-free under the null hypothesis but, as with these other classical methods, was only designed for univariate variables. Recent work of Weihs, Drton and Meinshausen (2017) has aimed to address some of computational challenges involved in extending these ideas to multivariate settings.
Recent research has focused on constructing tests that can be used for more complex data and that are consistent against wider classes of alternatives. The concept of distance covariance was introduced in Székely, Rizzo and Bakirov (2007) and can be expressed as a weighted $L_2$ norm between the characteristic function of the joint distribution and the product of the marginal characteristic functions. This concept has also been studied in high dimensions (Székely and Rizzo, 2013; Yao, Zhang and Shao, 2017), and for testing independence of several random vectors (Fan et al., 2017). In Sejdinovic et al. (2013) tests based on distance covariance were shown to be equivalent to a reproducing kernel Hilbert space (RKHS) test for a specific choice of kernel. RKHS tests have been widely studied in the machine learning community, with early understanding of the subject given by Bach and Jordan (2002) and Gretton et al. (2005), in which the Hilbert–Schmidt independence criterion was proposed. These tests are based on embedding the joint distribution and product of the marginal distributions into a Hilbert space and considering the norm of their difference in this space. One drawback of the kernel paradigm here is the computational complexity, though Jitkrittum, Szabó and Gretton (2016) and Zhang et al. (2017) have recently attempted to address this issue. The performance of these methods may also be strongly affected by the choice of kernel. In another line of work, there is a large literature on testing independence based on an empirical copula process; see for example Kojadinovic and Holmes (2009) and the references therein. Other test statistics include those based on partitioning the sample space (e.g. Gretton and Györfi, 2010; Heller et al., 2016). These have the advantage of being distribution-free under the null hypothesis, though their performance depends on the particular partition chosen.

We also remark that the basic independence testing problem has spawned many variants. For instance, Pfister et al. (2017) extend kernel tests to tests of mutual independence between a group of random vectors. Another important extension is to the problem of testing conditional independence, which is central to graphical modelling (Lauritzen, 1996) and also relevant to causal inference (Pearl, 2009). Existing tests of conditional independence include the proposals of Su and White (2008), Zhang et al. (2011) and Fan, Feng and Xia (2017).

To formalise the problem we consider, let $X$ and $Y$ have (Lebesgue) densities $f_X$ on $\mathbb{R}^{d_X}$ and $f_Y$ on $\mathbb{R}^{d_Y}$ respectively, and let $Z = (X,Y)$ have density $f$ on $\mathbb{R}^d$, where $d := d_X + d_Y$. Given independent and identically distributed copies $Z_1, \ldots, Z_n$ of $Z$, we wish to test the null hypothesis that $X$ and $Y$ are independent, denoted $H_0 : X \independent Y$, against the alternative that $X$ and $Y$ are not independent, written $H_1 : X \not\independent Y$. Our approach is based on constructing an estimator $\hat{I}_n = \hat{I}_n(Z_1, \ldots, Z_n)$ of the mutual information $I(X;Y)$ between
X and Y. Mutual information turns out to be a very attractive measure of dependence in this context; we review its definition and basic properties in Section 2 below. In particular, its decomposition into joint and marginal entropies (see (1) below) facilitates the use of recently-developed efficient entropy estimators derived from nearest neighbour distances (Berrett, Samworth and Yuan, 2017).

The next main challenge is to identify an appropriate critical value for the test. In the simpler setting where either of the marginals \( f_X \) and \( f_Y \) is known, a simulation-based approach can be employed to yield a test of any given size \( q \in (0, 1) \). We further provide regularity conditions under which the power of our test converges to 1 as \( n \to \infty \), uniformly over classes of alternatives with \( I(X;Y) \geq b_n \), say, where we may even take \( b_n = o(n^{-1/2}) \). To the best of our knowledge this is the first time that such a local power analysis has been carried out for an independence test for multivariate data. When neither marginal is known, we obtain our critical value via a permutation approach, again yielding a test of the nominal size. Here, under our regularity conditions, the test is uniformly consistent (has power converging to 1) against alternatives whose mutual information is bounded away from zero. We call our test MINT, short for Mutual Information Test; it is implemented in the \texttt{R} package \texttt{IndepTest} (Berrett, Grose and Samworth, 2017).

As an application of these ideas, we are able to introduce new goodness-of-fit tests of normal linear models based on assessing the independence of our vector of covariates and an appropriately-defined notion of an error vector. Such tests do not follow immediately from our earlier work, because we do not observe realisations of the error vector directly; instead, we only have access to residuals from a fitted model. Nevertheless, we are able to provide rigorous justification, again in the form of a local analysis, for our approach. It seems that, when fitting normal linear models, current standard practice in the applied statistics community for assessing goodness-of-fit is based on visual inspection of diagnostic plots such as those provided by the \texttt{plot} command in \texttt{R} when applied to an object of class \texttt{lm}. Our aim, then, is to augment the standard toolkit by providing a formal basis for inference regarding the validity of the model. Related work here includes Neumeyer (2009), Neumeyer and Van Keilegom (2010), Müller, Schick and Wefelmeyer (2012), Sen and Sen (2014) and Shah and Bühlmann (2017).

The remainder of the paper is organised as follows: after reviewing the concept of mutual information in Section 2.1, we explain in Section 2.2 how it can be estimated effectively from data using efficient entropy estimators. Our new tests, for the cases where one of the marginals is known and where they are both unknown, are introduced in Sections 3 and 4.
respectively. The regression setting is considered in Section 5, and numerical studies on both simulated and real data are presented in Section 6. Proofs are given in Section 7.

The following notation is used throughout. For a generic dimension \( D \in \mathbb{N} \), let \( \lambda_D \) and \( \| \cdot \| \) denote Lebesgue measure and the Euclidean norm on \( \mathbb{R}^D \) respectively. If \( f = d\mu/d\lambda_D \) and \( g = d\nu/d\lambda_D \) are densities on \( \mathbb{R}^D \) with respect to \( \lambda_D \), we write \( f \ll g \) if \( \mu \ll \nu \). For \( z \in \mathbb{R}^D \) and \( r \in [0, \infty) \), we write \( B_z(r) := \{ w \in \mathbb{R}^D : \| w - z \| \leq r \} \) and \( B_z^r := B_z(r) \setminus \{ z \} \).

We write \( \lambda_{\min}(A) \) for the smallest eigenvalue of a positive definite matrix \( A \), and \( \| B \|_F \) for the Frobenius norm of a matrix \( B \).

## 2 Mutual information

### 2.1 Definition and basic properties

Retaining our notation from the introduction, let \( Z := \{(x, y) : f(x, y) > 0\} \). A very natural measure of dependence is the mutual information between \( X \) and \( Y \), defined to be

\[
I(X; Y) = I(f) := \int_Z f(x, y) \log \frac{f(x, y)}{f_X(x) f_Y(y)} \, d\lambda_d(x, y),
\]

when \( f \ll f_X f_Y \), and defined to be \( \infty \) otherwise. This is the Kullback–Leibler divergence between the joint distribution of \((X, Y)\) and the product of the marginal distributions, so is non-negative, and equal to zero if and only if \( X \) and \( Y \) are independent. Another attractive feature of mutual information as a measure of dependence is that it is invariant to smooth, invertible transformations of \( X \) and \( Y \). Indeed, suppose that \( \mathcal{X} := \{ x : f_X(x) > 0 \} \) is an open subset of \( \mathbb{R}^{d_X} \) and \( \phi : \mathcal{X} \rightarrow \mathcal{X}' \) is a continuously differentiable bijection whose inverse \( \phi^{-1} \) has Jacobian determinant \( J(x') \) that never vanishes on \( \mathcal{X}' \). Let \( \Phi : \mathcal{X} \times \mathcal{Y} \rightarrow \mathcal{X}' \times \mathcal{Y} \) be given by \( \Phi(x, y) := (\phi(x), y) \), so that \( \Phi^{-1}(x', y) = (\phi^{-1}(x'), y) \) also has Jacobian determinant \( J(x') \). Then \( \Phi(X, Y) \) has density \( g(x', y) = f(\phi^{-1}(x'), y) |J(x')| \) on \( \Phi(Z) \) and \( X' = \phi(X) \) has density \( g_{X'}(x') = f_X(\phi^{-1}(x')) |J(x')| \) on \( \mathcal{X}' \). It follows that

\[
I(\phi(X); Y) = \int_{\Phi(Z)} g(x', y) \log \frac{g(x', y)}{g_{X'}(x') f_Y(y)} \, d\lambda_d(x', y)
= \int_{\Phi(Z)} g(x', y) \log \frac{f(\phi^{-1}(x'), y)}{f_X(\phi^{-1}(x')) f_Y(y)} \, d\lambda_d(x', y) = I(X; Y).
\]
This means that mutual information is nonparametric in the sense of Weihs, Drton and Meinshausen (2017), whereas several other measures of dependence, including distance covariance, RKHS measures and correlation-based notions are not in general. Under a mild assumption, the mutual information between $X$ and $Y$ can be expressed in terms of their joint and marginal entropies; more precisely, writing $Y := \{ y : f_Y(y) > 0 \}$, and provided that each of $H(X,Y)$, $H(X)$ and $H(Y)$ are finite,

$$I(X;Y) = \int_Z f \log f \, d\lambda - \int_X f_X \log f_X \, d\mu_X - \int_Y f_Y \log f_Y \, d\mu_Y$$

$$=: -H(X,Y) + H(X) + H(Y).$$

(1)

Thus, mutual information estimators can be constructed from entropy estimators.

Moreover, the concept of mutual information is easily generalised to more complex situations. For instance, suppose now that $(X,Y,W)$ has joint density $f$ on $\mathbb{R}^{d+w}$, and let $f_{(X,Y)|W}(\cdot|w)$, $f_{X|W}(\cdot|w)$ and $f_{Y|W}(\cdot|w)$ denote the joint conditional density of $(X,Y)$ given $W=w$ and the conditional densities of $X$ given $W=w$ and $Y$ given $W=w$ respectively. When $f_{(X,Y)|W}(\cdot|w) \ll f_{X|W}(\cdot|w)f_{Y|W}(\cdot|w)$ for each $w$ in the support of $W$, the conditional mutual information between $X$ and $Y$ given $W$ is defined as

$$I(X;Y|W) := \int_W f(x,y,w) \log \frac{f_{(X,Y)|W}(x,y|w)}{f_{X|W}(x|w)f_{Y|W}(y|w)} \, d\lambda_{d+w}(x,y,w),$$

where $W := \{(x,y,w) : f(x,y,w) > 0 \}$. This can similarly be written as

$$I(X;Y|W) = H(X,W) + H(Y,W) - H(X,Y,W) - H(W),$$

provided each of the summands is finite.

Finally, we mention that the concept of mutual information easily generalises to situations with $p$ random vectors. In particular, suppose that $X_1,\ldots,X_p$ have joint density $f$ on $\mathbb{R}^d$, where $d = d_1 + \ldots + d_p$ and that $X_j$ has marginal density $f_j$ on $\mathbb{R}^{d_j}$. Then, when $f \ll f_1 \ldots f_p$, and writing $X_p := \{(x_1,\ldots,x_p) \in \mathbb{R}^d : f(x_1,\ldots,x_p) > 0 \}$, we can define

$$I(X_1;\ldots;X_p) := \int_{X_p} f(x_1,\ldots,x_p) \log \frac{f(x_1,\ldots,x_p)}{f_1(x_1)\ldots f_p(x_p)} \, d\lambda_d(x_1,\ldots,x_p)$$

$$= \sum_{j=1}^p H(X_j) - H(X_1,\ldots,X_p),$$
with the second equality holding provided that each of the entropies is finite. The tests
we introduce in Sections 3 and 4 therefore extend in a straightforward manner to tests of
independence of several random vectors.

2.2 Estimation of mutual information

For \( i = 1, \ldots, n \), let \( Z_{(1),i}, \ldots, Z_{(n-1),i} \) denote a permutation of \( \{Z_1, \ldots, Z_n\} \setminus \{Z_i\} \) such that
\( \|Z_{(1),i} - Z_i\| \leq \ldots \leq \|Z_{(n-1),i} - Z_i\| \). For conciseness, we let
\[
\rho(k,i) := \|Z_{(k),i} - Z_i\|
\]
denote the distance between \( Z_i \) and the \( k \)th nearest neighbour of \( Z_i \). To estimate the
unknown entropies, we will use a weighted version of the Kozachenko–Leonenko estimator
(Kozachenko and Leonenko, 1987). For \( k = k^Z \in \{1, \ldots, n - 1\} \) and weights \( w_1^Z, \ldots, w_k^Z \)
satisfying \( \sum_{j=1}^{k} w_j^Z = 1 \), this is defined as
\[
\hat{H}_n^Z = \hat{H}_{n,k}^{d,w^Z}(Z_1, \ldots, Z_n) := \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} w_j^Z \log \left( \frac{\rho^d_{(j),i}}{V_d(n-1)} \right),
\]
where \( V_d := \frac{\pi^{d/2}}{\Gamma(1 + d/2)} \) denotes the volume of the unit \( d \)-dimensional Euclidean ball
and where \( \Psi \) denotes the digamma function. Berrett, Samworth and Yuan (2017) provided
conditions on \( k, w_1^Z, \ldots, w_k^Z \) and the underlying data generating mechanism under which \( \hat{H}_n^Z \)
is an efficient estimator of \( H(Z) \) (in the sense that its asymptotic normalised squared error
risk achieves the local asymptotic minimax lower bound) in arbitrary dimensions. With estimators \( \hat{H}_n^X \) and \( \hat{H}_n^Y \) of \( H(X) \) and \( H(Y) \) defined analogously as functions of \( (X_1, \ldots, X_n) \)
and \( (Y_1, \ldots, Y_n) \) respectively, we can use (1) to define an estimator of mutual information by
\[
\hat{I}_n = \hat{I}_n(Z_1, \ldots, Z_n) = \hat{H}_n^X + \hat{H}_n^Y - \hat{H}_n^Z.
\]
Having identified an appropriate mutual information estimator, we turn our attention in the
next two sections to obtaining appropriate critical values for our independence tests.
3 The case of one known marginal distribution

In this section, we consider the case where at least one of \(f_X\) and \(f_Y\) is known (in our experience, little is gained by knowledge of the second marginal density), and without loss of generality, we take the known marginal to be \(f_Y\). We further assume that we can generate independent and identically distributed copies of \(Y\), denoted \(\{Y_i^{(b)} : i = 1, \ldots, n, b = 1, \ldots, B\}\), independently of \(Z_1, \ldots, Z_n\). Our test in this setting, which we refer to as \text{MINTknown}\ (or \text{MINTknown}(q) when the nominal size \(q \in (0, 1)\) needs to be made explicit), will reject \(H_0\) for large values of \(\hat{I}_n\). The ideal critical value, if both marginal densities were known, would therefore be

\[
C_q(n) := \inf \{ r \in \mathbb{R} : P_{f_X f_Y}(\hat{I}_n > r) \leq q \}.
\]

Using our pseudo-data \(\{Y_i^{(b)} : i = 1, \ldots, n, b = 1, \ldots, B\}\), generated as described above, we define the statistics

\[
\hat{I}_n^{(b)} = \hat{I}_n((X_1, Y_1^{(b)}), \ldots, (X_n, Y_n^{(b)}))
\]

for \(b = 1, \ldots, B\). Motivated by the fact that these statistics have the same distribution as \(\hat{I}_n\) under \(H_0\), we can estimate the critical value \(C_q(n)\) by

\[
\hat{C}_q(n)^{(n),B} := \inf \left\{ r \in \mathbb{R} : \frac{1}{B+1} \sum_{b=0}^{B} \mathbb{1}_{\{\hat{I}_n^{(b)} \geq r\}} \leq q \right\},
\]

the \((1-q)\)th quantile of \(\{\hat{I}_n^{(0)}, \ldots, \hat{I}_n^{(B)}\}\), where \(\hat{I}_n^{(0)} := \hat{I}_n\). The following lemma justifies this critical value estimate.

**Lemma 1.** For any \(q \in (0, 1)\) and \(B \in \mathbb{N}\), the \text{MINTknown}(q) test that rejects \(H_0\) if and only if \(\hat{I}_n > \hat{C}_q(n)^{(n),B}\) has size at most \(q\), in the sense that

\[
\sup_{k \in \{1, \ldots, n-1\}} \sup_{(X,Y):I(X;Y)=0} \mathbb{P}(\hat{I}_n > \hat{C}_q(n)^{(n),B}) \leq q,
\]

where the inner supremum is over all joint distributions of pairs \((X, Y)\) with \(I(X;Y) = 0\).

An interesting feature of \text{MINTknown}, which is apparent from the proof of Lemma 1, is that there is no need to calculate \(\hat{H}_n^X\) in (1), either on the original data, or on the pseudo-data sets \(\{(X_1, Y_1^{(b)}), \ldots, (X_n, Y_n^{(b)}) : b = 1, \ldots, B\}\). This is because in the decomposition of the event \(\{\hat{I}_n^{(b)} \geq \hat{I}_n\}\) into entropy estimates, \(\hat{H}_n^X\) appears on both sides of the inequality, so it cancels. This observation somewhat simplifies our assumptions and analysis, as well as
reducing the number of tuning parameters that need to be chosen.

The remainder of this section is devoted to a rigorous study of the power of MINTknown that is compatible with a sequence of local alternatives \((f_n)\) having mutual information \(I_n \to 0\). To this end, we first define the classes of alternatives that we consider; these parallel the classes introduced by Berrett, Samworth and Yuan (2017) in the context of entropy estimation. Let \(\mathcal{F}_d\) denote the class of all density functions with respect to Lebesgue measure on \(\mathbb{R}^d\). For \(f \in \mathcal{F}_d\) and \(\alpha > 0\), let

\[
\mu_\alpha(f) := \int_{\mathbb{R}^d} \|z\|^\alpha f(z) \, dz.
\]

Now let \(\mathcal{A}\) denote the class of decreasing functions \(a : (0, \infty) \to [1, \infty)\) satisfying \(a(\delta) = o(\delta^{-\epsilon})\) as \(\delta \searrow 0\), for every \(\epsilon > 0\). If \(a \in \mathcal{A}\), \(\beta > 0\), \(f \in \mathcal{F}_d\) is \(m := \lceil \beta \rfloor - 1\)-times differentiable and \(z \in \mathcal{Z}\), we define

\[
r_a(z) := \left\{ \frac{8d^{1/2}a(f(z))}{2^{1/\beta}} \right\}^{-1/\beta}.
\]

The quantity \(M_{f,a,\beta}(z)\) measures the smoothness of derivatives of \(f\) in neighbourhoods of \(z\), relative to \(f(z)\) itself. Note that these neighbourhoods of \(z\) are allowed to become smaller when \(f(z)\) is small. Finally, for \(\Theta := (0, \infty)^4 \times \mathcal{A}\), and \(\theta = (\alpha, \beta, \nu, \gamma, a) \in \Theta\), let

\[
\mathcal{F}_{d,\theta} := \left\{ f \in \mathcal{F}_d : \mu_\alpha(f) \leq \nu, \|f\|_{\infty} \leq \gamma, \sup_{z : f(z) \geq \delta} M_{f,a,\beta}(z) \leq a(\delta) \ \forall \delta > 0 \right\}.
\]

Berrett, Samworth and Yuan (2017) show that all Gaussian and multivariate-\(t\) densities (amongst others) belong to \(\mathcal{F}_{d,\theta}\) for appropriate \(\theta \in \Theta\).

Now, for \(d_X, d_Y \in \mathbb{N}\) and \(\theta = (\theta, \theta_Y) \in \Theta^2\), define

\[
\mathcal{F}_{d_X, d_Y, \theta} := \left\{ f \in \mathcal{F}_{d_X + d_Y, \theta} : f_Y \in \mathcal{F}_{d_Y, \theta_Y}, f_X f_Y \in \mathcal{F}_{d_X + d_Y, \theta} \right\}
\]

and, for \(b \geq 0\), let

\[
\mathcal{F}_{d_X, d_Y, \theta}(b) := \left\{ f \in \mathcal{F}_{d_X, d_Y, \theta} : I(f) > b \right\}.
\]

Thus, \(\mathcal{F}_{d_X, d_Y, \theta}(b)\) consists of joint densities whose mutual information is greater than \(b\). In Theorem 2 below, we will show that for a suitable choice of \(b = b_n\) and for certain \(\theta \in \Theta^2\), the power of the test defined in Lemma 1 converges to 1, uniformly over \(\mathcal{F}_{d_X, d_Y, \theta}(b)\).

Before we can state this result, however, we must define the allowable choices of \(k\) and
the weight vectors. Given \( d \in \mathbb{N} \) and \( \theta = (\alpha, \beta, \gamma, \nu, a) \in \Theta \) let

\[
\tau_1(d, \theta) := \min \left\{ \frac{2\alpha}{5\alpha + 3d}, \frac{\alpha - d}{2\alpha}, \frac{4(\beta \wedge 1)}{4(\beta \wedge 1) + 3d} \right\}
\]

and

\[
\tau_2(d, \theta) := \min \left\{ 1 - \frac{d}{2\beta}, 1 - \frac{d/4}{\lfloor d/4 \rfloor + 1} \right\}
\]

Note that \( \min_{i=1,2} \tau_i(d, \theta) > 0 \) if and only if both \( \alpha > d \) and \( \beta > d/2 \). Finally, for \( k \in \mathbb{N} \), let

\[
\mathcal{W}(k) := \left\{ w = (w_1, \ldots, w_k)^T \in \mathbb{R}^k : \sum_{j=1}^k w_j \frac{\Gamma(j + 2\ell/d)}{\Gamma(j)} = 0 \text{ for } \ell = 1, \ldots, \lfloor d/4 \rfloor \right. \\
\left. \sum_{j=1}^k w_j = 1 \text{ and } w_j = 0 \text{ if } j \notin \{\lfloor k/d \rfloor, \lfloor 2k/d \rfloor, \ldots, k\} \right\}.
\]

Thus, our weights sum to 1; the other constraints ensure that the dominant contributions to the bias of the unweighted Kozachenko–Leonenko estimator cancel out to sufficiently high order, and that the corresponding \( j \)th nearest neighbour distances are not too highly correlated.

**Theorem 2.** Fix \( d_X, d_Y \in \mathbb{N} \), set \( d = d_X + d_Y \) and fix \( \vartheta = (\theta, \theta_Y) \in \Theta^2 \) with

\[
\min \left\{ \tau_1(d, \theta), \tau_1(d_Y, \theta_Y), \tau_2(d, \theta), \tau_2(d_Y, \theta_Y) \right\} > 0.
\]

Let \( k_0^* = k_{0,n}^*, k_Y^* = k_{Y,n}^* \) and \( k^* = k_n^* \) denote any deterministic sequences of positive integers with \( k_0^* \leq \min\{k_Y^*, k_n^*\} \), with \( k_0^*/\log^5 n \to \infty \) and with

\[
\max \left\{ \frac{k^*}{n^{\tau_1(d, \theta) - \epsilon}}, \frac{k_Y^*}{n^{\tau_1(d_Y, \theta_Y) - \epsilon}}, \frac{k^*}{n^{\tau_2(d, \theta)}}, \frac{k_Y^*}{n^{\tau_2(d_Y, \theta_Y)}} \right\} \to 0
\]

for some \( \epsilon > 0 \). Also suppose that \( w_Y = w_Y^{(k_Y)} \in \mathcal{W}(k_Y) \) and \( w = w^{(k)} \in \mathcal{W}(k) \), and that \( \limsup_n \max(\|w\|, \|w_Y\|) < \infty \). Then there exists a sequence \((b_n)\) such that \( b_n = o(n^{-1/2}) \) and with the property that for each \( q \in (0, 1) \) and any sequence \((B_n^*)\) with \( B_n^* \to \infty \),

\[
\inf_{B_n \geq B_n^*} \inf_{k \in \{k_0^*, \ldots, k_Y^*, k_n^*\}} \inf_{f \in F_{d_X, d_Y, \vartheta}(b_n)} \mathbb{P}_f (\hat{I}_n > \hat{C}_q^{(n)}(B_n)) \to 1.
\]

**Theorem 2** provides a strong guarantee on the ability of MINTknown to detect alternatives,
uniformly over classes whose mutual information is at least $b_n$, where we may even have $b_n = o(n^{-1/2})$.

4 The case of unknown marginal distributions

We now consider the setting in which the marginal distributions of both $X$ and $Y$ are unknown. Our test statistic remains the same, but now we estimate the critical value by permuting our sample in an attempt to mimic the behaviour of the test statistic under $H_0$. More explicitly, for some $B \in \mathbb{N}$, we propose independently of $(X_1, Y_1), \ldots, (X_n, Y_n)$ to simulate independent random variables $\tau_1, \ldots, \tau_B$ uniformly from $S_n$, the permutation group of $\{1, \ldots, n\}$, and for $b = 1, \ldots, B$, set $Z_i^{(b)} := (X_i, Y_{\tau_{b}(i)})$ and $\tilde{I}_n^{(b)} := \tilde{I}_n(Z_1^{(b)}, \ldots, Z_n^{(b)})$. For $q \in (0, 1)$, we can now estimate $C_q^{(n)}$ by

$$\hat{C}_q^{(n), B} := \inf \left\{ r \in \mathbb{R} : \frac{1}{B+1} \sum_{b=0}^{B} \mathbb{I}_{\{\tilde{I}_n^{(b)} \geq r\}} \leq q \right\},$$

where $\tilde{I}_n^{(0)} := \hat{I}_n$, and refer to the test that rejects $H_0$ if and only if $\hat{I}_n > \hat{C}_q^{(n), B}$ as MINTunknown($q$).

Lemma 3. For any $q \in (0, 1)$ and $B \in \mathbb{N}$, the MINTunknown($q$) test has size at most $q$:

$$\sup_{k \in \{1, \ldots, n-1\}} \sup_{(X,Y) : I(X;Y) = 0} \mathbb{P}(\hat{I}_n > \hat{C}_q^{(n), B}) \leq q.$$

Note that $\hat{I}_n > \hat{C}_q^{(n), B}$ if and only if

$$\frac{1}{B+1} \sum_{b=0}^{B} \mathbb{I}_{\{\tilde{I}_n^{(b)} \geq \hat{I}_n\}} \leq q. \quad (3)$$

This shows that estimating either of the marginal entropies is unnecessary to carry out the test, since $\tilde{I}_n^{(b)} - \hat{I}_n = \tilde{H}_n^{Z} - \tilde{H}_n^{(b)}$, where $\tilde{H}_n^{(b)} := \tilde{H}_{d,w,Z}^{\text{un}}(Z_1^{(b)}, \ldots, Z_n^{(b)})$ is the weighted Kozachenko–Leonenko joint entropy estimator based on the permuted data.

We now study the power of MINTunknown, and begin by introducing the classes of marginal densities that we consider. To define an appropriate notion of smoothness, for
\[ z \in \{ w : g(w) > 0 \} =: \mathcal{W}, \quad g \in \mathcal{F}_d \text{ and } \delta > 0, \quad \text{let} \]
\[ r_{z,g,\delta} := \left\{ \frac{\delta e^{\psi(k)}}{V_d(n-1)g(z)} \right\}^{1/d}. \quad (4) \]

Now, for \( A \) belonging to the class of Borel subsets of \( \mathcal{W} \), denoted \( \mathcal{B}(\mathcal{W}) \), define
\[ M_g(A) := \sup_{\delta \in (0,2]} \sup_{z \in A} \left| \frac{1}{V_d r_{z,g,\delta} g(z)} \int_{B_z(r_{z,g,\delta})} g \, d\lambda_d - 1 \right|. \]

Both \( r_{z,g,\delta} \) and \( M_g(\cdot) \) depend on \( n \) and \( k \), but for simplicity we suppress this in our notation.

Let \( \phi = (\alpha, \mu, \nu, (c_n), (p_n)) \in (0, \infty)^3 \times [0, \infty]^N \times [0, \infty)^N =: \Phi \) and define
\[ \mathcal{G}_{dX,dY,\phi} := \left\{ f \in \mathcal{F}_{dX+dY} : \max\{\mu_\alpha(f_X), \mu_\alpha(f_Y)\} \leq \mu, \quad \max\{\|f_X\|_\infty, \|f_Y\|_\infty\} \leq \nu, \right. \]
\[ \exists \mathcal{W}_n \in \mathcal{B}(\mathcal{X} \times \mathcal{Y}) \text{ s.t. } M_{f_X f_Y}(\mathcal{W}_n) \leq c_n, \quad \int_{\mathcal{W}_n} f_X f_Y \, d\lambda_d \leq p_n \quad \forall n \in \mathbb{N} \}. \]

In addition to controlling the \( \alpha \)th moment and uniform norms of the marginals \( f_X \) and \( f_Y \), the class \( \mathcal{G}_{d,\phi} \) asks for there to be a (large) set \( \mathcal{W}_n \) on which this product of marginal densities is uniformly well approximated by a constant over small balls. This latter condition is satisfied by products of many standard parametric families of marginal densities, including normal, Weibull, Gumbel, logistic, gamma, beta, and \( t \) densities, and is what ensures that nearest neighbour methods are effective in this context.

The corresponding class of joint densities we consider, for \( \phi = (\alpha, \mu, \nu, (c_n), (p_n)) \in \Phi \), is
\[ \mathcal{H}_{d,\phi} := \left\{ f \in \mathcal{F}_d : \mu_\alpha(f) \leq \mu, \quad \|f\|_\infty \leq \nu, \right. \]
\[ \exists \mathcal{Z}_n \in \mathcal{B}(\mathcal{Z}) \text{ s.t. } M_f(\mathcal{Z}_n) \leq c_n, \quad \int_{\mathcal{Z}_n} f \, d\lambda_d \leq p_n \quad \forall n \in \mathbb{N} \}. \]

In many cases, we may take \( \mathcal{Z}_n = \{ z : f(z) \geq \delta_n \} \), for some appropriately chosen sequence \( (\delta_n) \) with \( \delta_n \to 0 \) as \( n \to \infty \). For instance, suppose we fix \( d \in \mathbb{N} \) and \( \theta = (\alpha, \beta, \nu, \gamma, a) \in \Theta \). Then, by Berrett, Samworth and Yuan (2017, Lemma 12), there exists such a sequence \( (\delta_n) \), as well as sequences \( (c_n) \) and \( (p_n) \), where
\[ \delta_n = \frac{ka(k/(n-1))^{3d/2}}{n-1} \log(n-1), \quad c_n = \frac{15}{7} \frac{2^{3/2}}{d (\beta \wedge 1)} \log^{-\beta_\wedge 1} (n-1), \]
for large $n$ and $p_n = o((k/n)^{\alpha/n^\epsilon})$ for every $\epsilon > 0$, such that $\mathcal{F}_{d,\theta} \subseteq \mathcal{H}_{d,\phi}$ with $\phi = (\alpha, \mu, \nu, (c_n), (p_n)) \in \Phi$. We are now in a position to state our main result on the power of MINTunknown.

**Theorem 4.** Let $d_X, d_Y \in \mathbb{N}$, let $d = d_X + d_Y$ and fix $\phi = (\alpha, \mu, \nu, (c_n), (p_n)) \in \Phi$ with $c_n \to 0$ and $p_n = o(1/\log n)$ as $n \to \infty$. Let $k_0^* = k_0^{*,n}$ and $k_1^* = k_1^{*,n}$ denote two deterministic sequences of positive integers satisfying $k_0^* \leq k_1^*$, $k_0^*/\log^2 n \to \infty$ and $(k_1^* \log^2 n)/n \to 0$. Then for any $b > 0$, $q \in (0, 1)$ and any sequence $(B_n^*)$ with $B_n^* \to \infty$ as $n \to \infty$,

$$
\inf_{B_n \geq B_n^*} \inf_{k \in \{k_0^{*,n}, \ldots, k_1^{*,n}\}} \inf_{f \in \mathcal{G}_{d_X, d_Y, \phi} \cap \mathcal{H}_{d, \phi}} \mathbb{P}(\hat{I}_n > \tilde{C}_q^{(n), B_n}) \to 1
$$

as $n \to \infty$.

Theorem 4 shows that MINTunknown is uniformly consistent against a wide class of alternatives.

### 5 Regression setting

In this section we aim to extend the ideas developed above to the problem of goodness-of-fit testing in linear models. Suppose we have independent and identically distributed pairs $(X_1, Y_1), \ldots, (X_n, Y_n)$ taking values in $\mathbb{R}^p \times \mathbb{R}$, with $\mathbb{E}(Y_i^2) < \infty$ and $\mathbb{E}(X_1 X_1^T)$ finite and positive definite. Then

$$
\beta_0 := \arg\min_{\beta \in \mathbb{R}^p} \mathbb{E}\{(Y_1 - X_1^T \beta)^2\}
$$

is well-defined, and we can further define $\epsilon_i := Y_i - X_i^T \beta_0$ for $i = 1, \ldots, n$. We show in the proof of Theorem 6 below that $\mathbb{E}(\epsilon_1 X_1) = 0$, but for the purposes of interpretability and inference, it is often convenient if the random design linear model

$$
Y_i = X_i^T \beta_0 + \epsilon_i, \quad i = 1, \ldots, n,
$$

holds with $X_i$ and $\epsilon_i$ independent. A goodness-of-fit test of this property amounts to a test of $H_0 : X_1 \perp \perp \epsilon_1$ against $H_1 : X_1 \not\perp \perp \epsilon_1$. The main difficulty here is that $\epsilon_1, \ldots, \epsilon_n$ are not observed directly. Given an estimator $\hat{\beta}$ of $\beta_0$, the standard approach for dealing with this problem is to compute residuals $\tilde{\epsilon}_i := Y_i - X_i^T \hat{\beta}$ for $i = 1, \ldots, n$, and use these as a proxy for $\epsilon_1, \ldots, \epsilon_n$. Many introductory statistics textbooks, e.g. Dobson (2002, Section 2.3.4), Dalgaard (2002, Section 5.2) suggest examining for patterns plots of residuals against fitted
values, as well as plots of residuals against each covariate in turn, as a diagnostic, though it is difficult to formalise this procedure. (It is also interesting to note that when applying the `plot` function in R to an object of type `lm`, these latter plots of residuals against each covariate in turn are not produced, presumably because it would be prohibitively time-consuming to check them all in the case of many covariates.)

The naive approach based on our work so far is simply to use the permutation test of Section 4 on the data \((X_1, \hat{\epsilon}_1), \ldots, (X_n, \hat{\epsilon}_n)\). Unfortunately, calculating the test statistic \(\hat{I}_n\) on permuted data sets does not result in an exchangeable sequence, which makes it difficult to ensure that this test has the nominal size \(q\). To circumvent this issue, we assume that the marginal distribution of \(\epsilon_1\) under \(H_0\) has \(\mathbb{E}(\epsilon_1) = 0\) and is known up to a scale factor \(\sigma^2 := \mathbb{E}(\epsilon_1^2)\); in practice, it will often be the case that this marginal distribution is taken to be \(N(0, \sigma^2)\), for some unknown \(\sigma > 0\). We also assume that we can sample from the density \(f_\eta\) of \(\eta_1 := \epsilon_1/\sigma\); of course, this is straightforward in the normal distribution case above. Let \(X = (X_1 \cdots X_n)^T, Y = (Y_1, \ldots, Y_n)^T\), and suppose the vector of residuals \(\hat{\epsilon} := (\hat{\epsilon}_1, \ldots, \hat{\epsilon}_n)^T\) is computed from the least squares estimator \(\hat{\beta} := (X^TX)^{-1}X^TY\). We then define standardised residuals by \(\hat{\eta}_i := \hat{\epsilon}_i/\hat{\sigma}\), for \(i = 1, \ldots, n\), where \(\hat{\sigma}^2 := n^{-1}\|\hat{\epsilon}\|^2\); these standardised residuals are invariant under changes of scale of \(\epsilon := (\epsilon_1, \ldots, \epsilon_n)^T\). Suppressing the dependence of our entropy estimators on \(k\) and the weights \(w_1, \ldots, w_k\) for notational simplicity, our test statistic is now given by

\[
\hat{I}^{(0)}_n := \hat{H}^p_n(X_1, \ldots, X_n) + \hat{H}^1_n(\hat{\eta}_1, \ldots, \hat{\eta}_n) - \hat{H}^{p+1}_n((X_1, \hat{\eta}_1), \ldots, (X_n, \hat{\eta}_n)).
\]

Writing \(\eta := \epsilon/\sigma\), we note that

\[
\hat{\eta}_i = \frac{1}{\hat{\sigma}}(Y_i - X_i^T\hat{\beta}) = \frac{1}{\hat{\sigma}}\left\{\epsilon_i - X_i^T(\hat{\beta} - \beta_0)\right\} = \frac{n^{1/2}\eta_i - X_i^T(X^TX)^{-1}X^T\eta}{\|\eta - X^T(X^TX)^{-1}X^T\eta\|},
\]

whose distribution does not depend on the unknown \(\beta_0\) or \(\sigma^2\). Let \(\{\eta^{(b)} = (\eta^{(b)}_1, \ldots, \eta^{(b)}_n)^T : b = 1, \ldots, B\}\) denote independent random vectors, whose components are generated independently from \(f_\eta\). For \(b = 1, \ldots, B\) we then set \(\hat{\sigma}^{(b)} := n^{-1/2}\|\hat{\eta}^{(b)}\|\) and, for \(i = 1, \ldots, n\), let

\[
\hat{\eta}^{(b)}_i := \frac{1}{\hat{\sigma}^{(b)}}\left\{\eta^{(b)}_i - X_i^T(X^TX)^{-1}X^T\eta^{(b)}\right\}.
\]

We finally compute

\[
\hat{I}^{(b)}_n := \hat{H}^p_n(X_1, \ldots, X_n) + \hat{H}^1_n(\hat{\eta}^{(b)}_1, \ldots, \hat{\eta}^{(b)}_n) - \hat{H}^{p+1}_n((X_1, \hat{\eta}_1^{(b)}), \ldots, (X_n, \hat{\eta}_n^{(b)})).
\]
Analogously to our development in Sections 3 and 4, we can then define a critical value by
\[ \bar{C}_q^{(n),B} := \inf \left\{ r \in \mathbb{R} : \frac{1}{B+1} \sum_{b=0}^{B} \mathbb{I}(\hat{I}_n^{(b)} \geq r) \leq q \right\}. \]

Conditional on \( X \) and under \( H_0 \), the sequence \((\hat{I}_n^{(0)}, \ldots, \hat{I}_n^{(B)})\) is independent and identically distributed and unconditionally it is an exchangeable sequence under \( H_0 \). This is the crucial observation from which we can immediately derive that the resulting test has the nominal size.

**Lemma 5.** For each \( q \in (0,1) \) and \( B \in \mathbb{N} \), the MINTregression\((q)\) test that rejects \( H_0 \) if and only if \( \hat{I}_n^{(0)} > \bar{C}_q^{(n),B} \) has size at most \( q \):
\[
\sup_{k \in \{1, \ldots, n-1\}} \sup_{(X,Y) : I(X;Y) = 0} \mathbb{P}(\hat{I}_n > \bar{C}_q^{(n),B}) \leq q.
\]

As in previous sections, we are only interested in the differences \( \hat{I}_n^{(0)} - \hat{I}_n^{(b)} \) for \( b = 1, \ldots, B \), and in these differences, the \( \tilde{H}_n^p(X_1, \ldots, X_n) \) terms cancel out, so these marginal entropy estimators need not be computed.

In fact, to simplify our power analysis, it is more convenient to define a slightly modified test, which also has the nominal size. Specifically, we assume for simplicity that \( m := n/2 \) is an integer, and consider a test in which the sample is split in half, with the second half of the sample used to calculate the estimators \( \tilde{\beta}_2 \) and \( \tilde{\sigma}^2_2 \) of \( \beta_0 \) and \( \sigma^2 \) respectively. On the first half of the sample, we calculate
\[
\hat{\eta}_{i,(1)} := \frac{Y_i - X_i^T \tilde{\beta}_2}{\tilde{\sigma}_2}
\]
for \( i = 1, \ldots, m \) and the test statistic
\[
\hat{I}_n^{(0)} := \tilde{H}_n^p(X_1, \ldots, X_m) + \tilde{H}_n^1(\hat{\eta}_{1,(1)}, \ldots, \hat{\eta}_{m,(1)}) - \tilde{H}_n^{p+1}(X_1, \hat{\eta}_{1,(1)}, \ldots, X_m, \hat{\eta}_{m,(1)}).
\]

Corresponding estimators \( \{\hat{I}_n^{(b)} : b = 1, \ldots, B\} \) based on the simulated data may also be computed using the same sample-splitting procedure, and we then obtain the critical value \( \bar{C}_q^{(n),B} \) in the same way as above. The advantage from a theoretical perspective of this approach is that, conditional on \( \tilde{\beta}_2 \) and \( \tilde{\sigma}^2_2 \), the random variables \( \hat{\eta}_{1,(1)}, \ldots, \hat{\eta}_{m,(1)} \) are independent and identically distributed.
To describe the power properties of MINTregression, we first define several densities: for \( \gamma \in \mathbb{R}^p \) and \( s > 0 \), let \( f_{\hat{\eta}^{\gamma,s}}^{\gamma,s} \) and \( f_{\hat{\eta}^{(1),\gamma,s}}^{\gamma,s} \) denote the densities of \( \hat{\eta}_1^{\gamma,s} := (\eta_1 - X_1^T \gamma)/s \) and \( \hat{\eta}_1^{(1),\gamma,s} := (\eta_1^{(1)} - X_1^T \gamma)/s \) respectively; further, let \( f_{X,\hat{\eta}}^{\gamma,s} \) and \( f_{X,\hat{\eta}^{(1)}}^{\gamma,s} \) be the densities of \( (X, \hat{\eta}_1^{\gamma,s}) \) and \( (X, \hat{\eta}_1^{(1),\gamma,s}) \) respectively. Note that imposing assumptions on these densities amounts to imposing assumptions on the joint density \( f \) of \( (X, \epsilon) \). For \( \Omega := \Theta \times \Theta \times (0, \infty) \times (0, 1) \times (0, \infty) \times (0, \infty) \), and \( \omega = (\theta_1, \theta_2, r_0, s_0, \Lambda, \lambda_0) \), we therefore let \( \mathcal{F}_{p+1,\omega}^* \) denote the class of joint densities \( f \) of \( (X, \epsilon) \) satisfying the following three requirements:

(i) \[
\left\{ f_{\hat{\eta}^{\gamma,s}}^{\gamma,s} : \gamma \in B_0(r_0), s \in [s_0, 1/s_0] \right\} \cup \left\{ f_{\hat{\eta}^{(1),\gamma,s}}^{\gamma,s} : \gamma \in B_0(r_0), s \in [s_0, 1/s_0] \right\} \subseteq \mathcal{F}_{1,\theta_1}
\]
and

(ii) \[
\sup_{\gamma \in B_0(r_0)} \max \left\{ \mathbb{E} \log^2 f_{\hat{\eta}^{\gamma,1}}^{\gamma,1}(\eta_1), \mathbb{E} \log^2 f_{\hat{\eta}^{(1),\gamma,1}}^{\gamma,1}(\eta_1) \right\} \leq \Lambda,
\]

and

(iii) Writing \( \Sigma := \mathbb{E}(X_1X_1^T) \), we have \( \lambda_{\min}(\Sigma) \geq \lambda_0 \).

The first of these requirements ensures that we can estimate efficiently the marginal entropy of our scaled residuals, as well as the joint entropy of these scaled residuals and our covariates. The second condition is a moment condition that allows us to control \( |H(\eta_1 - X_1^T \gamma) - H(\eta_1)| \) (and similar quantities) in terms of \( \|\gamma\| \), when \( \gamma \) belongs to a small ball around the origin. To illustrate the second part of this condition, it is satisfied, for instance, if \( f_\eta \) is a standard normal density and \( \mathbb{E}(\|X_1\|^4) < \infty \), or if \( f_\eta \) is a t density and \( \mathbb{E}(\|X_1\|^\alpha) < \infty \) for some \( \alpha > 0 \); the first part of the condition is a little more complicated but similar. The final condition is very natural for random design regression problems.

By the same observation on the sequence \( (\hat{I}^{(0)}_n, \ldots, \hat{I}^{(B)}_n) \) as was made regarding the sequence \( (\hat{I}^{(0)}_n, \ldots, \hat{I}^{(B)}_n) \) just before Lemma 5, we see that the sample-splitting version of the MINTregression\((q)\) test has size at most \( q \).

**Theorem 6.** Fix \( p \in \mathbb{N} \) and \( \omega = (\theta_1, \theta_2, r_0, s_0, \Lambda, \lambda_0) \in \Omega \), where the first component of \( \theta_2 \) is
\( \alpha_2 \geq 4 \) and the second component of \( \theta_1 \) is \( \beta_1 \geq 1 \). Assume that

\[
\min\left\{ \tau_1(1, \theta_1), \tau_1(p + 1, \theta_2), \tau_2(1, \theta_1), \tau_2(p + 1, \theta_2) \right\} > 0.
\]

Let \( k^*_0 = k^*_{0, n}, k^*_\eta = k^*_{\eta, n} \) and \( k^* = k^*_n \) denote any deterministic sequences of positive integers with \( k^*_0 \leq \min\{k^*_\eta, k^*\} \), with \( k^*_n/\log^5 n \to \infty \) and with

\[
\max\left\{ \frac{k^*_\eta}{n^{\tau_1(p + 1, \theta_2) - \epsilon}}, \frac{k^*}{n^{\tau_1(1, \theta_1) - \epsilon}}, \frac{k^*}{n^{\tau_2(p + 1, \theta_2)}}, \frac{k^*_\eta}{n^{\tau_2(1, \theta_1)}} \right\} \to 0
\]

for some \( \epsilon > 0 \). Also suppose that \( w_\eta = w^{(k_n)}_\eta \in W^{(k_n)} \) and \( w = w^{(k)} \in W^{(k)} \), and that \( \limsup_n \max(\|w\|, \|w_\eta\|) < \infty \). Then for any sequence \( (b_n) \) such that \( n^{1/2} b_n \to \infty \), any \( q \in (0, 1) \) and any sequence \( (B_n) \) with \( B_n \to \infty \),

\[
\inf_{B_n \geq B_{\eta, n}, k_\eta \in \{k^*_0, \ldots, k^*_\eta\}} \inf_{f \in \mathcal{F}_{1, p+1} : I(f) \geq b_n} \mathbb{P}_f(\hat{I}_n > \hat{C}^{(n)}_{\eta, B_n}) \to 1.
\]

Finally in this section, we consider partitioning our design matrix as \( X = (X^* X^{**}) \in \mathbb{R}^{n \times (p_0 + p_1)} \), with \( p_0 + p_1 = p \), and describe an extension of \textsc{MINTregression} to cases where we are interested in testing the independence between \( \epsilon \) and \( X^* \). For instance, \( X^{**} \) may consist of an intercept term, or transformations of variables in \( X^* \), as in the real data example presented in Section 6.3 below. Our method for simulating standardised residual vectors \( \{\hat{\eta}^{(b)} : b = 1, \ldots, B\} \) remains unchanged, but our test statistic and corresponding null statistics become

\[
\hat{I}^{(0)}_n := \hat{H}^{p}_n(X^1_1, \ldots, X^*_n) + \hat{H}^{1}_n(\hat{\eta}_1, \ldots, \hat{\eta}_n) - \hat{H}^{p+1}_n((X^*_1, \hat{\eta}_1), \ldots, (X^*_n, \hat{\eta}_n))
\]

\[
\hat{I}^{(b)}_n := \hat{H}^{p}_n(X^1_1, \ldots, X^*_n) + \hat{H}^{1}_n(\hat{\eta}^{(b)}_1, \ldots, \hat{\eta}^{(b)}_n) - \hat{H}^{p+1}_n((X^*_1, \hat{\eta}^{(b)}_1), \ldots, (X^*_n, \hat{\eta}^{(b)}_n)), \quad b = 1, \ldots, B.
\]

The sequence \( (\hat{I}^{(0)}_n, \hat{I}^{(1)}_n, \ldots, \hat{I}^{(B)}_n) \) is again exchangeable under \( H_0 \), so a \textit{p}-value for this modified test is given by

\[
\frac{1}{B + 1} \sum_{b = 0}^{B} \mathbbm{1}_{\{\hat{I}^{(b)}_n \geq \hat{I}^{(0)}_n\}}.
\]
6 Numerical studies

6.1 Practical considerations

For practical implementation of the MINTunknown test, we consider both a direct, data-driven approach to choosing \( k \), and a multiscale approach that averages over a range of values of \( k \). To describe the first method, let \( K \subseteq \{1, \ldots, n-1\} \) denote a plausible set of values of \( k \). For a given \( N \in \mathbb{N} \) and independently of the data, generate \( \tau_1, \ldots, \tau_{2N} \) independently and uniformly from \( S_n \), and for each \( k \in K \) and \( j = 1, \ldots, 2N \) let \( \hat{H}_{n,k}^{(j)} \) be the (unweighted) Kozachenko–Leonenko joint entropy estimate with tuning parameter \( k \) based on the sample \( \{(X_i, Y_{\tau_j(i)}) : i = 1, \ldots, n\} \). We may then choose

\[
\hat{k} := \text{sargmin}_{k \in K} \sum_{j=1}^{N} (\hat{H}_{n,k}^{(2j)} - \hat{H}_{n,k}^{(2j-1)})^2,
\]

where sargmin denotes the smallest index of the argmin in the case of a tie. In our simulations below, which use \( N = 100 \), we refer to the resulting test as MINTauto.

For our multiscale approach, we again let \( K \subseteq \{1, \ldots, n-1\} \) and, for \( k \in K \), let \( \hat{h}^{(0)}(k) := \hat{H}_{n,k} \) denote the (unweighted) Kozachenko–Leonenko entropy estimate with tuning parameter \( k \) based on the original data \( (X_1, Y_1), \ldots, (X_n, Y_n) \). Now, for \( b = 1, \ldots, B \) and \( k \in K \), we let \( \tilde{h}^{(b)}(k) := \tilde{H}_{n,(k)}^{(b)} \) denote the Kozachenko–Leonenko entropy estimate with tuning parameter \( k \) based on the permuted data \( Z_1^{(b)}, \ldots, Z_n^{(b)} \). Writing \( \bar{h}^{(b)} := |K|^{-1} \sum_{k \in K} \tilde{h}^{(b)}(k) \) for \( b = 0, 1, \ldots, B \), we then define the \( p \)-value for our test to be

\[
\frac{1}{B+1} \sum_{b=0}^{B} 1_{\{\bar{h}^{(0)} \geq \bar{h}^{(b)}\}}.
\]

By the exchangeability of \( (\bar{h}^{(0)}, \bar{h}^{(1)}, \ldots, \bar{h}^{(B)}) \) under \( H_0 \), the corresponding test has the nominal size. We refer to this test as MINTav, and note that if \( K \) is taken to be a singleton set then we recover MINTunknown. In our simulations below, we took \( K = \{1, \ldots, 20\} \) and \( B = 100 \).

6.2 Simulated data

To study the empirical performance of our methods, we first compare our tests to existing approaches through their performance on simulated data. For comparison, we present cor-
responding results for a test based on the empirical copula process described by Kojadinovic and Holmes (2009) and implemented in the R package copula (Hofert et al., 2017), a test based on the HSIC implemented in the R package dHSIC (Pfister and Peters, 2017), a test based on the distance covariance implemented in the R package energy (Rizzo and Szekely, 2017) and the improvement of Hoeffding’s test described in Bergsma and Dassios (2014) and implemented in the R package TauStar (Weihs, Drton and Leung, 2016). We also present results for an oracle version of our tests, denoted simply as MINT, which for each parameter value in each setting, uses the best (most powerful) choice of \( k \). Throughout, we took \( q = 0.05 \) and \( n = 200 \), ran 5000 repetitions for each parameter setting, and for our comparison methods, used the default tuning parameter values recommended by the corresponding authors. We consider three classes of data generating mechanisms, designed to illustrate different possible types of dependence:

(i) For \( l \in \mathbb{N} \) and \((x, y) \in [-\pi, \pi]^2\), define the density function

\[
f_l(x, y) = \frac{1}{\pi^2} \{1 + \sin(lx) \sin(ly)\}.
\]

This class of densities, which we refer to as sinusoidal, are identified by Sejdinovic et al. (2013) as challenging ones to detect dependence, because as \( l \) increases, the dependence becomes increasingly localised, while the marginal densities are uniform on \([-\pi, \pi]\) for each \( l \). Despite this, by the periodicity of the sine function, we have that the mutual information does not depend on \( l \): indeed,

\[
I(f_l) = \frac{1}{\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \{1 + \sin(lx) \sin(ly)\} \log(1 + \sin(lx) \sin(ly)) \, dx \, dy \\
= \frac{1}{\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} (1 + \sin u \sin v) \log(1 + \sin u \sin v) \, du \, dv \approx 0.0145.
\]

(ii) Let \( L, \Theta, \epsilon_1, \epsilon_2 \) be independent with \( L \sim U(\{1, \ldots, l\}) \) for some parameter \( l \in \mathbb{N} \), \( \Theta \sim U[0, 2\pi] \), and \( \epsilon_1, \epsilon_2 \sim N(0, 1) \). Set \( X = L \cos \Theta + \epsilon_1/4 \) and \( Y = L \sin \Theta + \epsilon_2/4 \).

For large values of \( l \), the distribution of \((X/l, Y/l)\) approaches the uniform distribution on the unit disc.

(iii) Let \( X, \epsilon \) be independent with \( X \sim U[-1, 1] \), \( \epsilon \sim N(0, 1) \), and for a parameter \( \rho \in [0, \infty) \), let \( Y = |X|^{\rho} \epsilon \).

For each of these three classes of data generating mechanisms, we also consider a corre-
sponding multivariate setting in which we wish to test the independence of $X$ and $Y$ when $X = (X_1, X_2)^T, Y = (Y_1, Y_2)^T$. Here, $(X_1, Y_1), X_2, Y_2$ are independent, with $X_1$ and $Y_1$ having the dependence structures described above, and $X_2, Y_2 \sim U(0, 1)$. In these multivariate settings, the generalisations of the TauStar test were too computationally intensive, so were omitted from the comparison.

The results are presented in Figure 1(a). Unsurprisingly, there is no uniformly most powerful test among those considered, and if the form of the dependence were known in advance, it may well be possible to design a tailor-made test with good power. Nevertheless, Figure 1(a) shows that, especially in the first and second of the three settings described above, the MINT and MINTav approaches have very strong performance. In these examples, the dependence becomes increasingly localised as $l$ increases, and the flexibility to choose a smaller value of $k$ in such settings means that MINT approaches are particularly effective. Where the dependence is more global in nature, such as in setting (iii), other approaches may be better suited, though even here, MINT is competitive. Interestingly, the multiscale MINTav appears to be much more effective than the MINTauto approach of choosing a single value of $k$; indeed, in setting (iii), MINTav even outperforms the oracle choice of $k$.

### 6.3 Real data

In this section we illustrate the use of MINTregression on a data set comprising the average minimum daily January temperature, between 1931 and 1960 and measured in degrees Fahrenheit, in 56 US cities, indexed by their latitude and longitude (Peixoto, 1990). Fitting a normal linear model to the data with temperature as the response and latitude and longitude as covariates leads to the diagnostic plots shown in Figures 2(a) and 2(b). Based on these plots, it is relatively difficult to assess the strength of evidence against the model. Centering all of the variables and running MINTregression with $k_\eta = 6, k = 3$ and $B = 1785 = \lfloor 10^5/56 \rfloor$ yielded a $p$-value of 0.00224, providing strong evidence that the normal linear model is not a good fit to the data. Further investigation is possible via partial regression: in Figure 2(c) we plot residuals based on a simple linear fit of Temperature on Latitude against the residuals of another linear fit of Longitude on Latitude. This partial regression plot is indicative of a cubic relationship between Temperature and Longitude after removing the effects of Latitude. Based on this evidence we fitted a new model with a quadratic and cubic term in Longitude added to the first model. The $p$-value of the resulting $F$-test was $< 2.2 \times 10^{-16}$, giving overwhelming evidence in favour of the inclusion of the quadratic and cubic terms. We then ran our extension of MINTregression to test the independence of $\epsilon$
Figure 1: Power curves for the different tests considered, for settings (i) (left), (ii) (middle) and (iii) (right). The marginals are univariate (top) and bivariate (bottom).

Figure 2: Plots of residuals against fitted values (left) and square roots of the absolute values of the standardised residuals against fitted values (middle) for the US cities temperature data. The right panel gives a partial regression plot after removing the effect of latitude from both the response and longitude.
and (Longitude, Latitude), as described at the end of Section 5 with $B = 1000$. This resulted in a $p$-value of 0.0679, so we do not reject this model at the 5% significance level.

7 Proofs

7.1 Proofs from Section 3

Proof of Lemma 1. Under $H_0$, the finite sequence $(\hat{I}_n, \hat{I}_n^{(1)}, \ldots, \hat{I}_n^{(B)})$ is exchangeable. It follows that under $H_0$, if we split ties at random, then every possible ordering of $\hat{I}_n, \hat{I}_n^{(1)}, \ldots, \hat{I}_n^{(B)}$ is equally likely. In particular, the (descending order) rank of $\hat{I}_n$ among $\{\hat{I}_n, \hat{I}_n^{(1)}, \ldots, \hat{I}_n^{(B)}\}$, denoted rank($\hat{I}_n$), is uniformly distributed on $\{1, 2, \ldots, B + 1\}$. We deduce that for any $k \in \{1, \ldots, n - 1\}$ and writing $P_{H_0}$ for the probability under the product of any marginal distributions for $X$ and $Y$,

$$P_{H_0}(\hat{I}_n > \hat{C}_q^{(n),B}) = P_{H_0}\left(\frac{1}{B + 1} \sum_{b=0}^{B} \mathbb{I}_{\{\hat{I}_n^{(b)} \geq \hat{I}_n\}} \leq q\right)$$

$$\leq P_{H_0}(\text{rank}(\hat{I}_n) \leq q(B + 1)) = \frac{q(B + 1)}{B + 1} \leq q,$$

as required. 

Let $V(f) := \text{Var} \log \frac{f(X,Y)}{f_X(x)f_Y(y)}$. The following result will be useful in the proof of Theorem 2.

Lemma 7. Fix $d_X, d_Y \in \mathbb{N}$ and $\vartheta \in \Theta^2$. Then

$$\sup_{f \in F_{d_X, d_Y, \vartheta(0)}} \frac{V(f)}{I(f)^{1/4}} < \infty.$$ 

Proof of Lemma 7. For $x \in \mathbb{R}$ we write $x_- := \max(0, -x)$. We have

$$\mathbb{E}\left[\left\{\log \frac{f(X,Y)}{f_X(X)f_Y(Y)}\right\}^-\right] = \int_{\{(x,y): f(x,y) \leq f_X(x)f_Y(y)\}} f(x,y) \log \frac{f_X(x)f_Y(y)}{f(x,y)} \ d\lambda_d(x,y)$$

$$\leq \int_{\{(x,y): f(x,y) \leq f_X(x)f_Y(y)\}} f(x,y) \left\{\frac{f_X(x)f_Y(y)}{f(x,y)} - 1\right\} \ d\lambda_d(x,y)$$

$$= \sup_{A \in B(\mathbb{R}^d)} \left\{\int_A f_X f_Y - \int_A f\right\} \leq \{I(f)/2\}^{1/2},$$
where the final inequality is Pinsker's inequality. We therefore have that

\[ V(f) \leq \mathbb{E} \log^2 \frac{f(X, Y)}{f_X(X)f_Y(Y)} = \mathbb{E} \left\{ \left| \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right|^{1/2} \right\} \left\{ \left| \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right|^{3/2} \right\} \]

\[ \leq \left\{ \mathbb{E} \left| \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right| \right\}^{1/2} \left\{ \mathbb{E} \left| \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right|^{3/2} \right\} \]

\[ = \left( I(f) + 2\mathbb{E} \left\{ \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right\} \right)^{1/2} \left\{ \mathbb{E} \left| \log \frac{f(X, Y)}{f_X(X)f_Y(Y)} \right|^{3/2} \right\}^{1/2} \]

\[ \leq 2\left\{ I(f) + 2^{1/2} I(f)^{1/2} \right\} \left\{ \mathbb{E} \left| \log (f_X(X)f_Y(Y)) \right|^3 + \mathbb{E} \left| \log f(X, Y) \right|^3 \right\}^{1/2}. \]

By Berrett, Samworth and Yuan (2017, Lemma 11(i)), we conclude that

\[ \sup_{f \in \mathcal{F}_{dX,dY,\vartheta}} \frac{V(f)}{I(f)^{1/4}} < \infty. \]

The result follows from this fact, together with the observation that

\[ \sup_{f \in \mathcal{F}_{dX,dY,\vartheta}} V(f) \leq 2 \sup_{f \in \mathcal{F}_{dX,dY,\vartheta}} \left\{ \mathbb{E} \log^2 f(X, Y) + \mathbb{E} \log^2 (f_X(X)f_Y(Y)) \right\} < \infty, \quad (7) \]

where the final bound follows from another application of Berrett, Samworth and Yuan (2017, Lemma 11(i)).

**Proof of Theorem 2.** Fix \( f \in \mathcal{F}_{dX,dY,\vartheta}(b_n) \). We have by two applications of Markov's inequality that

\[ \mathbb{P}_f(\tilde{I}_n \leq \tilde{C}_q^{(n),b_n}) \leq \frac{1}{q(B_n + 1)} \{ 1 + B_n \mathbb{P}_f(\tilde{I}_n^{(1)} \geq \tilde{I}_n) \} \]

\[ \leq \frac{1}{q} \mathbb{P}_f(\{ \tilde{I}_n - \tilde{I}_n^{(1)} \geq I(f) \}) + \frac{1}{q(B_n + 1)} \]

\[ \leq \frac{1}{q I(f)^2} \mathbb{E}_f[(\tilde{I}_n - \tilde{I}_n^{(1)} - I(f))^2] + \frac{1}{q(B_n + 1)} \quad (8) \]

It is convenient to define the following entropy estimators based on pseudo-data, as well as oracle versions of our entropy estimators: let \( Z_i^{(1)} := (X_i^T, Y_i^{(1)}T) \), \( Z^{(1)} := (Z_1^{(1)}, \ldots, Z_n^{(1)})^T \)
and \( Y(1) := (Y_1^{(1)}, \ldots, Y_n^{(1)})^T \) and set

\[
\begin{align*}
\hat{H}_{n,k}^Z(1) := \hat{H}_{n,k}^Z(Z^{(1)}), & \quad \hat{H}_{n,k}^Y(1) := \hat{H}_{n,k}^Y(Y^{(1)}) \\
H_n^* := -\frac{1}{n} \sum_{i=1}^n \log f(X_i, Y_i), & \quad H_n^* := -\frac{1}{n} \sum_{i=1}^n \log f_Y(Y_i), \\
H_n^{*,(1)} := -\frac{1}{n} \sum_{i=1}^n \log f_X(X_i) f_Y(Y_i^{(1)}), & \quad H_n^{*,Y(1)} := -\frac{1}{n} \sum_{i=1}^n \log f_Y(Y_i^{(1)}).
\end{align*}
\]

Writing \( I_n^* := \frac{1}{n} \sum_{i=1}^n \log \frac{f(X_i, Y_i)}{f_X(X_i) f_Y(Y_i)} \) we have by Berrett, Samworth and Yuan (2017, Theorem 1) that

\[
\sup_{k_Y \in \{k_0^*, \ldots, k_Y^*\}} \sup_{f \in \mathcal{F}_{d_X, d_Y, \vartheta}} n \mathbb{E}_f \left\{ (\hat{I}_n - \hat{I}^{(1)}_n - I^*_n)^2 \right\} = \sup_{k_Y \in \{k_0^*, \ldots, k_Y^*\}} \sup_{f \in \mathcal{F}_{d_X, d_Y, \vartheta}} \mathbb{E}_f \left\{ \left( \hat{H}_n^Y - \hat{H}_n - \hat{H}_n^{Y(1)} + \hat{H}_n^{(1)} - \left( H_n^{*,Y} - H_n^* - H_n^{*,Y(1)} + H_n^{*,(1)} \right) \right)^2 \right\} \leq 4n \sup_{k_Y \in \{k_0^*, \ldots, k_Y^*\}} \sup_{f \in \mathcal{F}_{d_X, d_Y, \vartheta}} \mathbb{E}_f \left\{ \left( \hat{H}_n^Y - H_n^{*,Y} \right)^2 + \left( \hat{H}_n - H_n^* \right)^2 + \left( \hat{H}_n^{(1)} - H_n^{*,Y(1)} \right)^2 + \left( \hat{H}_n^{(1)} - H_n^{*,(1)} \right)^2 \right\} \to 0.
\]

It follows by Cauchy–Schwarz and the fact that \( \mathbb{E}\left[ \left\{ I_n^* - I(f) \right\}^2 \right] = V(f)/n \) that

\[
\begin{align*}
\epsilon_n^2 := \sup_{k_Y \in \{k_0^*, \ldots, k_Y^*\}} \sup_{f \in \mathcal{F}_{d_X, d_Y, \vartheta}} \left| n \mathbb{E}_f \left\{ (\hat{I}_n - \hat{I}^{(1)}_n - I(f))^2 \right\} - V(f) \right| \\
\leq \sup_{k_Y \in \{k_0^*, \ldots, k_Y^*\}} \sup_{f \in \mathcal{F}_{d_X, d_Y, \vartheta}} \left\{ n \mathbb{E}_f \left\{ (\hat{I}_n - \hat{I}^{(1)}_n - I^*_n)^2 \right\} + 2 \left[ n \mathbb{E}_f \left\{ (\hat{I}_n - \hat{I}^{(1)}_n - I^*_n)^2 \right\} V(f) \right]^{1/2} \right\} \\
\to 0,
\end{align*}
\]

where we use (7) to bound \( V(f) \) above. Now consider \( b_n := \max(\epsilon_n^{1/2} n^{-1/2}, n^{-4/7} \log n) \).
By (8), (9) and Lemma 7 we have that

\[
\inf_{B_n \geq B_n^*} \inf_{k_Y \in \{k_0^*,\ldots,k_Y^*\}} \inf_{f \in \mathcal{F}_{dX,dY,\varrho}(b_n)} \mathbb{P}(\hat{I}_n > C_q(n),B_n) \\
\geq 1 - \sup_{k_Y \in \{k_0^*,\ldots,k_Y^*\}} \sup_{f \in \mathcal{F}_{dX,dY,\varrho}(b_n)} \mathbb{E}_f(\{\hat{I}_n - \hat{I}_n^{(1)} - I(f)\}^2) - \frac{1}{q(B_n^* + 1)} \\
\geq 1 - \sup_{f \in \mathcal{F}_{dX,dY,\varrho}(b_n)} \frac{V(f) + \epsilon_n^2}{nqI(f)^2} - \frac{1}{q(B_n^* + 1)} \\
\geq 1 - \frac{1}{q \log^{7/4} n} \sup_{f \in \mathcal{F}_{dX,dY,\varrho}(0)} \frac{V(f)}{I(f)^{1/4}} - \frac{\epsilon_n}{q} - \frac{1}{q(B_n^* + 1)} \rightarrow 1,
\]

as required. \(\square\)

### 7.2 Proofs from Section 4

**Proof of Lemma 3.** We first claim that \((\hat{I}_n^{(0)}, \hat{I}_n^{(1)}, \ldots, \hat{I}_n^{(B)})\) is an exchangeable sequence under \(H_0\). Indeed, let \(\sigma\) be an arbitrary permutation of \(\{0, 1, \ldots, B\}\), and recall that \(\hat{I}_n^{(b)}\) is computed from \((X_i, Y_{\tau(b)(i)})_{i=1}^n\), where \(\tau(b)\) is uniformly distributed on \(S_n\). Note that, under \(H_0\), we have \((X_i, Y_i)_{i=1}^n \overset{d}{=} (X_i, Y_{\tau(i)}(i))_{i=1}^n\) for any \(\tau \in S_n\). Hence, for any \(A \in \mathcal{B}(\mathbb{R}^{B+1})\),

\[
\mathbb{P}_{H_0}(\\(\hat{I}_n^{(\sigma(0))}, \ldots, \hat{I}_n^{(\sigma(B))}) \in A) \\
= \frac{1}{(n!)^B} \sum_{\pi_1, \ldots, \pi_B \in S_n} \mathbb{P}_{H_0}(\\(\hat{I}_n^{(\sigma(0))}, \ldots, \hat{I}_n^{(\sigma(B))}) \in A|\tau_1 = \pi_1, \ldots, \tau_B = \pi_B) \\
= \frac{1}{(n!)^B} \sum_{\pi_1, \ldots, \pi_B \in S_n} \mathbb{P}_{H_0}(\\(\hat{I}_n^{(0)}, \ldots, \hat{I}_n^{(B)}) \in A|\tau_1 = \pi_{\sigma(1)}\pi_{\sigma(0)}, \ldots, \tau_B = \pi_{\sigma(B)}\pi_{\sigma(0)}) \\
= \mathbb{P}_{H_0}(\\(\hat{I}_n^{(0)}, \ldots, \hat{I}_n^{(B)}) \in A).
\]

By the same argument as in the proof of Lemma 1 we now have that

\[
\mathbb{P}_{H_0}(\hat{I}_n > \tilde{C}_q(n),B) \leq \frac{\lfloor q(B + 1) \rfloor}{B + 1} \leq q,
\]

as required. \(\square\)

Recall the definition of \(\hat{H}_n^{(1)}\) given just after (3). We give the proof of Theorem 4 below, followed by Lemma 8, which is the key ingredient on which it is based.
Proof of Theorem 4. We have by Markov’s inequality that
\[
\mathbb{P}_f(\hat{I}_n \leq \tilde{C}_q^{(n)}, B_n) \leq \frac{1}{q(B_n + 1)} \{1 + B_n \mathbb{P}_f(\hat{I}_n \leq \tilde{I}_n^{(1)})\} \leq \frac{1}{q} \mathbb{P}_f(\hat{H}_n^Z \geq \hat{H}_n^{(1)}) + \frac{1}{q(B_n + 1)}.
\]
(10)

But
\[
\mathbb{P}_f(\hat{H}_n^Z \geq \hat{H}_n^{(1)}) = \mathbb{P}_f(\hat{H}_n^Z - H(X, Y) \geq \hat{H}_n^{(1)} - H(X) - H(Y) + I(X; Y))
\]
\[
\leq \mathbb{P}(|\hat{H}_n^Z - H(X, Y)| \geq \frac{1}{2} I(X; Y)) + \mathbb{P}(|\hat{H}_n^{(1)} - H(X) - H(Y)| \geq \frac{1}{2} I(X; Y))
\]
\[
\leq \frac{2}{I(X; Y)} \{\mathbb{E}|\hat{H}_n^Z - H(X, Y)| + \mathbb{E}|\hat{H}_n^{(1)} - H(X) - H(Y)|\}.
\]
(11)
The theorem therefore follows immediately from (10), (11) and Lemma 8 below. 

Lemma 8. Let $d_X, d_Y \in \mathbb{N}$, let $d = d_X + d_Y$ and fix $\phi = (\alpha, \mu, \nu, (c_n), (p_n)) \in \Phi$ with $c_n \to 0$ and $p_n = o(1/\log n)$ as $n \to \infty$. Let $k_0^* = k_{0,n}^*$ and $k_1^* = k_{1,n}^*$ denote two deterministic sequences of positive integers satisfying $k_0^* \leq k_1^*$, $k_0^*/\log^2 n \to \infty$ and $(k_1^*/\log^2 n)/n \to 0$.

Then
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in G_{d_X, d_Y, \phi}} \mathbb{E}_f|\hat{H}_n^{(1)} - H(X) - H(Y)| \to 0,
\]
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in H_{d, \phi}} \mathbb{E}_f|\hat{H}_n^Z - H(X, Y)| \to 0
\]
as $n \to \infty$.

Proof. We prove only the first claim in Lemma 8, since the second claim involves similar arguments but is more straightforward because the estimator is based on an independent and identically distributed sample and no permutations are involved. Throughout this proof, we write $a \lesssim b$ to mean that there exists $C > 0$, depending only on $d_X, d_Y \in \mathbb{N}$ and $\phi \in \Phi$, such that $a \leq Cb$. Fix $f \in G_{d_X, d_Y, \phi}$, where $\phi = (\alpha, \mu, \nu, (c_n), (p_n))$. Write $\rho_{(k),i,(1)}$ for the distance from $Z_i^{(1)}$ to its $k$th nearest neighbour in the sample $Z_1^{(1)}, \ldots, Z_n^{(1)}$ and $\xi_i^{(1)} := e^{-\Psi(k)}V_0(n - 1)\rho_{(k),i,(1)}^2$ so that
\[
\hat{H}_n^{(1)} = \frac{1}{n} \sum_{i=1}^n \log \xi_i^{(1)}.
\]
Recall that $S_n$ denotes the set of all permutations of $\{1, \ldots, n\}$, and define $S_n' \subseteq S_n$ to be the
set of permutations that fix \( \{1, \ldots, l\} \) and have no fixed points among \( \{l + 1, \ldots, n\} \); thus \(|S^l_n| = (n-l)! \sum_{r=0}^{n-l} (-1)^r / r! \). For \( \tau \in S_n \), write \( \mathbb{P}_\tau(\cdot) := \mathbb{P}(\cdot | \tau_1 = \tau) \), and \( \mathbb{E}_\tau(\cdot) := \mathbb{E}(\cdot | \tau_1 = \tau) \). Let \( l_n := \lfloor \log \log n \rfloor \). For \( i = 1, \ldots, n \), let

\[
A'_i := \{ \text{The } k \text{ nearest neighbours of } Z^{(1)}_i \text{ are among } Z^{(1)}_{l+1}, \ldots, Z^{(1)}_n \},
\]

and let \( A_i := A'_i \cap \{ Z^{(1)}_i \in \mathcal{W}_n \} \). Using the exchangeability of \( \xi^{(1)}_1, \ldots, \xi^{(1)}_n \), our basic decomposition is as follows:

\[
\mathbb{E}|\hat{H}^{(1)}_n - H(X) - H(Y)|
\leq \frac{1}{n!} \sum_{l=0}^{l_n} \binom{n}{l} \sum_{\tau \in S^l_n} \left\{ \frac{1}{n} \sum_{i=1}^{l} \mathbb{E}_\tau|\log \xi^{(1)}_i| + \mathbb{E}_\tau \left| \frac{1}{n} \sum_{i=l+1}^{n} \log \xi^{(1)}_i - H(X) - H(Y) \right| \right\}
\leq \frac{1}{n!} \sum_{l=0}^{l_n} \binom{n}{l} \sum_{\tau \in S^l_n} \left\{ \frac{1}{n} \sum_{i=1}^{l} \mathbb{E}_\tau|\log \xi^{(1)}_i| + \mathbb{E}_\tau \left| \frac{1}{n} \sum_{i=l+1}^{n} \log \xi^{(1)}_i \right| \mathbb{1}_{A_i} - H(X) - H(Y) \right| \right\}
\leq \frac{1}{n} \sum_{i=l+1}^{n} \mathbb{E}_\tau\left| \log \xi^{(1)}_i \right| \mathbb{1}_{(A'_i \setminus (A'_i)^c) \cup (A_i)^c} \right) \right\} + \frac{1}{n!} \sum_{l=0}^{l_n} \binom{n}{l} \sum_{\tau \in S^l_n} \mathbb{E}_\tau\left| \hat{H}^{(1)}_n \right| + |H(X) + H(Y)| \right) \right).
\]

(12)

The rest of the proof consists of handling each of these four terms.

**Step 1:** We first show that

\[
\sup_{k \in \{1, \ldots, n-1\}} \sup_{f \in \mathcal{G}_{d_X,d_Y,f}} \frac{1}{n!} \sum_{l=l_n+1}^{n} \binom{n}{l} \sum_{\tau \in S^l_n} \mathbb{E}_\tau\left| \hat{H}^{(1)}_n \right| + |H(X) + H(Y)| \right) \right) \rightarrow 0
\]

(13)
as \( n \rightarrow \infty \). Writing \( \rho^{(k),i,X} \) for the distance from \( X_i \) to its \( k \)th nearest neighbour in the sample \( X_1, \ldots, X_n \) and defining \( \rho^{(k),i,Y} \) similarly, we have

\[
\max\{\rho^{2(k),i,X}, \rho^{2(k),\tau_1(i),Y}\} \leq \rho^{2(k),i,1} \leq \rho^{2(n-1),i,X} \leq \rho^{2(n-1),\tau_1(i),Y}.
\]
Using the fact that \( \log(a + b) \leq \log 2 + |\log a| + |\log b| \) for \( a, b > 0 \), we therefore have that

\[
\begin{align*}
|\log \xi_i^{(1)}| & \leq \left| \log \left( \frac{V_d(n-1)}{e^{\Psi(k)}} \right) \right| + d \log \rho_{(k),i,X} + \frac{d}{2} \log \left( \frac{\rho_{(k),i,(1)}}{\rho_{(k),i,X}} \right) \\
& \leq \left| \log \left( \frac{V_d(n-1)}{e^{\Psi(k)}} \right) \right| + 2d \log \rho_{(k),i,X} + \frac{d}{2} \log 2 + d \log \rho_{(n-1),i,X} + d \log \rho_{(n-1),\tau_1(i),Y} \\
& \leq \left| \log \left( \frac{V_d(n-1)}{e^{\Psi(k)}} \right) \right| + \frac{d}{2} \log 2 \\
& \quad + 4d \max_{j=1,...,n} \max \{-\log \rho_{(1),j,X}, -\log \rho_{(1),j,Y}, \log \rho_{(n-1),j,X}, \log \rho_{(n-1),j,Y}\}. \quad (14)
\end{align*}
\]

Now, by the triangle inequality, a union bound and Markov’s inequality,

\[
\begin{align*}
\mathbb{E}\left\{ \max_{j=1,...,n} \log \rho_{(n-1),j,X} \right\} - \log 2 & \leq \mathbb{E} \left[ \log \left( \max_{j=1,...,n} \|X_j\| \right) \right] \leq \mathbb{E}\left[ \left\{ \log \left( \max_{j=1,...,n} \|X_j\| \right) \right\}_+ \right] \\
& = \int_0^\infty \mathbb{P}\left( \max_{j=1,...,n} \|X_j\| \geq e^M \right) dM \\
& \leq \frac{1}{\alpha} \max \{0, \log n + \log \mathbb{E}(\|X_1\|^\alpha)\} + \frac{1}{\alpha} n \mathbb{E}(\|X_1\|^\alpha) \exp\left\{ -\log n - \log \mathbb{E}(\|X_1\|^\alpha) \right\} \\
& \leq \frac{1}{\alpha} \left\{ 1 + \log n + \max(0, \log \mu) \right\}, \quad (16)
\end{align*}
\]

and the same bound holds for \( \mathbb{E}\max_{j=1,...,n} \log \rho_{(n-1),j,Y} \). Similarly,

\[
\begin{align*}
\mathbb{E}\left\{ \min_{j=1,...,n} \log \rho_{(1),j,X} \right\}_- & = \int_0^\infty \mathbb{P}\left( \min_{j=1,...,n} \rho_{(1),j,X} \leq e^{-M} \right) dM \\
& \leq 2d_X^{-1} \log n + n(n-1)V_{d_X} \|f_X\|_\infty \int_0^\infty e^{-Mdx} dM \\
& \leq 2d_X^{-1} \log n + d_X^{-1}V_{d_X} \nu, \quad (17)
\end{align*}
\]

and the same bound holds for \( \mathbb{E}\left[ \left\{ \min_{j=1,...,n} \log \rho_{(1),j,Y} \right\}_- \right] \) once we replace \( d_X \) with \( d_Y \). By (15), (16), (17) and Stirling’s approximation,

\[
\begin{align*}
\sum_{l=l_n+1}^n \binom{n}{l} & \binom{n}{l} \max_{k=1,...,n-1} \sup_{f \in \mathcal{G}_{d_X,d_Y,\phi}} \mathbb{E}(\hat{H}_n^{(1)}|1_{\{\tau_1 \in S_n^l\}}) \leq \log n \sum_{l=l_n+1}^n \binom{n}{l} \mathbb{P}(\tau_1 \in S_n^l) \\
& \leq \frac{\log n}{n!} \binom{n}{l_n+1} (n-l_n-1)! = \frac{\log n}{(l_n+1)!} \leq \frac{\log n}{\sqrt{2\pi} (l_n+1)} \left( \frac{e}{l_n+1} \right)^{l_n+1} \to 0 \quad (18)
\end{align*}
\]
as \( n \to \infty \). Moreover, for any \( f \in \mathcal{G}_{dX,dY,\phi} \) and \((X,Y) \sim f\), writing \( \epsilon = \alpha/(\alpha + 2d_X) \),

\[
|H(X)| \leq \int_X f_X |\log f_X| \leq \int_X f_X(x) \log \left( \frac{f_X(x)}{f_X(x)} \right) \, dx + |\log f_X| \\
\leq \frac{\|f_X\|_\infty}{\epsilon} \int_X f_X(x)^{1-\epsilon} \, dx + |\log f_X| \\
\leq \frac{\nu^\epsilon}{\epsilon} (1 + \mu)^{1-\epsilon} \left\{ \int_{\mathbb{R}^d_X} (1 + \|x\|^\alpha)^{-\frac{1-\epsilon}{\epsilon}} \, dx \right\}^\epsilon \\
+ \max \left\{ \log \nu, \frac{1}{\alpha} \log \left( \frac{V^\alpha_{dX} \mu^{dX} (\alpha + d_X)^{\alpha + d_X}}{\alpha^{dX}} \right) \right\},
\]

(19)

where the lower bound on \( \|f_X\|_\infty \) is due to the fact that \( V^\alpha_{dX} \mu^{dX} (\alpha + d_X)^{\alpha + d_X} \geq \alpha^{dX} \) by Berrett, Samworth and Yuan (2017, Lemma 10(i)). Combining (19) with the corresponding bound on \( H(Y) \), as well as (18), we deduce that (13) holds.

**Step 2:** We observe that by (15), (16) and (17),

\[
\sup_{k \in \{1, \ldots, n-1\}} \sup_{f \in \mathcal{G}_{dX,dY,\phi}} \frac{1}{n!} \sum_{l=0}^{l_n} \binom{n}{l} \sum_{\tau \in S^l_n} \frac{1}{n} \sum_{i=1}^{l} \mathbb{E}_\tau \left| \log \xi^{(1)}_i \right| \lesssim \frac{l_n \log n}{n} \to 0.
\]

(20)

**Step 3:** We now show that

\[
\sup_{k \in \{k^*_0, \ldots, k^*_1\}} \sup_{f \in \mathcal{G}_{dX,dY,\phi}} \frac{1}{n!} \sum_{l=0}^{l_n} \binom{n}{l} \sum_{\tau \in S^l_n} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_\tau \left( \left| \log \xi_i^{(1)} 1_{(A_i^\tau \setminus (A_i^\tau)\cup (A_i^\tau))} \right| \right) \to 0.
\]

(21)

We use an argument that involves covering \( \mathbb{R}^d \) by cones; cf. Biau and Devroye (2015, Section 20.7). For \( w_0 \in \mathbb{R}^d, z \in \mathbb{R}^d \setminus \{0\} \) and \( \theta \in [0, \pi] \), define the cone of angle \( \theta \) centred at \( w_0 \) in the direction \( z \) by

\[
C(w_0, z, \theta) := w_0 + \{ w \in \mathbb{R}^d \setminus \{0\} : \cos^{-1}(z^T w/(\|z\| \|w\|)) \leq \theta \} \cup \{0\}.
\]

By Biau and Devroye (2015, Theorem 20.15), there exists a constant \( C_{\pi/6} \in \mathbb{N} \) depending only on \( d \) such that we may cover \( \mathbb{R}^d \) by \( C_{\pi/6} \) cones of angle \( \pi/6 \) centred at \( Z_1^{(1)} \). In each cone, mark the \( k \) nearest points to \( Z_1^{(1)} \) among \( Z_2^{(1)}, \ldots, Z_n^{(1)} \). Now fix a point \( Z_i^{(1)} \) that is not marked and a cone that contains it, and let \( Z_{i_1}^{(1)}, \ldots, Z_{i_k}^{(1)} \) be the \( k \) marked points in this
cone. By Biau and Devroye (2015, Lemma 20.5) we have, for each \( j = 1, \ldots, k \), that

\[
\| Z_i^{(1)} - Z_{ij}^{(1)} \| < \| Z_i^{(1)} - Z_1^{(1)} \|. 
\]

Thus, \( Z_1^{(1)} \) is not one of the \( k \) nearest neighbours of the unmarked point \( Z_i^{(1)} \), and only the marked points, of which there are at most \( kC_{\pi/6} \), may have \( Z_1^{(1)} \) as one of their \( k \) nearest neighbours. This immediately generalises to show that at most \( klC_{\pi/6} \) of the points \( Z_{i+1}^{(1)}, \ldots, Z_n^{(1)} \) may have any of \( Z_1^{(1)}, \ldots, Z_l^{(1)} \) among their \( k \) nearest neighbours. Then, by (15), (16) and (17), we have that, uniformly over \( k \in \{1, \ldots, n - 1\} \),

\[
\sup_{f \in \mathcal{G}_{d_X,d_Y,\phi}} \max_{\tau \in \mathcal{U}_{[0,s]}^n} \frac{1}{n} \mathbb{E}_\tau \left( \sum_{i=l+1}^n \log \xi_i^{(1)} | \mathbb{I}_{(A_i^c)} \right) \leq \frac{kl_n}{n} \log n. \quad (22)
\]

Now, for \( x \in \mathcal{X} \) and \( r \in [0, \infty) \), let \( h_x(r) := \int_{B_x(r)} f_x \) and, for \( s \in [0, 1) \), let \( h_x^{-1}(s) := \inf \{ r \geq 0 : h_x(r) \geq s \} \). We also write \( B_{k,n-k}(s) := \frac{\Gamma(n)}{\Gamma(k)\Gamma(n-k)} s^{k-1} (1-s)^{n-k-1} \) for \( s \in (0,1) \).

Then, by (4) and (13) in Berrett, Samworth and Yuan (2017), there exists \( C > 0 \), depending only on \( d_X \) and \( \phi \), such that, uniformly for \( k \in \{1, \ldots, n - 1\} \),

\[
\max_{i=1+1, \ldots, n} \mathbb{E}_\tau \left\{ \log \rho(k,i,X) | \mathbb{I}_{\{ Z_i^{(1)} \in \mathcal{W}_n^c \}} \right\} 
\leq \int_{\mathcal{W}_n^c} f_X(x)f_Y(y) \int_0^1 \log \left( \frac{V_{d_X}(n-1)h_x^{-1}(s)}{e^{r(k)}} \right) \left| B_{k,n-k}(s) \right| ds d\lambda_d(x,y)
\leq \int_{\mathcal{W}_n^c} f_X(x)f_Y(y) \int_0^1 \{ \log n - \log s - \log(1-s) + \log(1+C\|x\|) \} B_{k,n-k}(s) ds d\lambda_d(x,y). \quad (23)
\]

Now, given \( \epsilon \in (0,1) \), by Hölder’s inequality, and with \( K_\epsilon := \max\{1, (\epsilon\alpha - 1) \log 2, C^{\alpha}\} / (\epsilon\alpha) \),

\[
\int_{\mathcal{W}_n^c} f_X(x)f_Y(y) \log(1+C\|x\|) d\lambda_d(x,y) \leq K_\epsilon \int_{\mathcal{W}_n^c} f_X(x)f_Y(y) (1 + \|x\|^{\alpha}) d\lambda_d(x,y)
\leq K_\epsilon \left\{ \int_{\mathcal{W}_n^c} f_X(x)f_Y(y) (1 + \|x\|^{\alpha}) d\lambda_d(x,y) \right\}^{1-\epsilon} \left\{ \int_{\mathcal{W}_n^c} f_X(x)f_Y(y) d\lambda_d(x,y) \right\}^{\epsilon}
\leq K_\epsilon (1 + \mu)^{\epsilon} p_0^{1-\epsilon}. \quad (24)
\]

We deduce from (23) and (24) that for each \( \epsilon \in (0,1) \) and uniformly for \( k \in \{1, \ldots, n - 1\} \),

\[
\max_{l+1=1, \ldots, n} \sup_{f \in \mathcal{G}_{d_X,d_Y,\phi}} \mathbb{E}_\tau \left\{ \log \rho(k,i,X) | \mathbb{I}_{\{ Z_i^{(1)} \in \mathcal{W}_n^c \}} \right\} \lesssim p_n \log n + K_\epsilon p_0^{1-\epsilon}.
\]

30
From similar bounds on the corresponding terms with $\rho_{(k),i,X}$ replaced with $\rho_{(n-1),i,X}$ and $\rho_{(n-1),r_i(X),Y}$, we conclude from (14) that for every $\epsilon \in (0, 1)$ and uniformly for $k \in \{1, \ldots, n-1\}$,

$$\max_{i=l+1, \ldots, n} \sup_{f \in G_{d_X,d_Y,\phi}} \mathbb{E}_r \{ \log \xi_i^{(1)} \mathbb{1}_{\{Z_i^{(1)} \in W_n^\epsilon\}} \} \lesssim p_n \log n + K_1 p_n^{1-\epsilon}. \quad (25)$$

The claim (21) follows from (22) and (25).

**Step 4:** Finally, we show that

$$\sup_{k \in \{k_0, \ldots, k_1\}} \sup_{f \in G_{d_X,d_Y,\phi}} \frac{1}{n} \sum_{l=0}^n \left( \frac{n}{l} \right) \sum_{\tau \in S_n} \mathbb{E}_r \left[ \frac{1}{n} \sum_{i=l+1}^n (\log \xi_i^{(1)}) \mathbb{1}_{A_i} - H(X) - H(Y) \right] \to 0. \quad (26)$$

To this end, we consider the following further decomposition:

$$\mathbb{E}_r \left[ \frac{1}{n} \sum_{i=l+1}^n (\log \xi_i^{(1)}) \mathbb{1}_{A_i} - H(X) - H(Y) \right] \leq \frac{1}{n} \sum_{i=l+1}^n \mathbb{E}_r \left[ (\log \xi_i^{(1)} f_X f_Y (Z_i^{(1)})) \mathbb{1}_{A_i} \right] + \frac{1}{n} \mathbb{E}_r \left[ \sum_{i=l+1}^n \left( \log f_X f_Y (Z_i^{(1)}) \right) \mathbb{1}_{\{A_i \cap (A_i')^c \cup (A_i')^c\}} \right]$$

$$+ \mathbb{E}_r \left[ \frac{1}{n} \sum_{i=l+1}^n \log f_X f_Y (Z_i^{(1)}) - \frac{n-l}{n} \{H(X) + H(Y)\} \right] + \frac{l}{n} \{H(X) + H(Y)\}. \quad (27)$$

We deal first with the second term in (27). Now, by the arguments in Step 3,

$$\frac{1}{n} \mathbb{E}_r \left[ \sum_{i=l+1}^n \left( \log f_X f_Y (Z_i^{(1)}) \right) \mathbb{1}_{(A_i')^c} \right] \leq \frac{C_{\sigma/6} k_1 l}{n} \max_{i=l+1, \ldots, n} \{ \log f_X (X_i) \}$$

$$\leq \frac{C_{\sigma/6} k_1 l}{n} \left\{ \mathbb{E} \left( \max_{i=l+1, \ldots, n} |\log f_X (X_i)| \right) + \mathbb{E} \left( \max_{i=l+1, \ldots, n} |\log f_Y (Y_i)| \right) \right\}. \quad (28)$$

Now, for any $s > 0$, by Hölder’s inequality,

$$\mathbb{P} \{ f_X (X_1) \leq s \} \leq s^{2(\alpha + d_X)} \int_{x : f(x) \leq s} f_X (x)^{1 - \frac{\alpha}{2(\alpha + d_X)}} \, dx$$

$$\leq s^{2(\alpha + d_X)} (1 + \mu)^{1 - \frac{\alpha}{2(\alpha + d_X)}} \left\{ \int_{\mathbb{R}^d_X} \frac{1}{(1 + \|x\|^{\alpha + 2d_X})^{\alpha}} \, dx \right\}^{\frac{\alpha}{2(\alpha + d_X)}} =: \tilde{K}_{d_X,\phi} s^{\frac{\alpha}{2(\alpha + d_X)}}.$$
Writing \( t_\ast := -\frac{2(\alpha + d_X)}{\alpha} \log(n - l) \), we deduce that for \( n \geq 3 \),
\[
\mathbb{E}\left( \max_{i=l+1, \ldots, n} | \log f_X(X_i) | \right) \leq \log \nu - \mathbb{E}\left( \min_{i=l+1, \ldots, n} \log f_X(X_i) \right)
\leq \log \nu + (n - l) \tilde{K}_{d_X, \phi} \int_{-\infty}^{t_\ast} e^{\frac{\alpha t}{\alpha + d_X}} dt + \frac{2(\alpha + d_X)}{\alpha} \log n
= \log \nu + \frac{2(\alpha + d_X)}{\alpha} \tilde{K}_{d_X, \phi} + \frac{2(\alpha + d_X)}{\alpha} \log n.
\] (29)

Combining (29) with the corresponding bound on \( \mathbb{E}\left( \max_{i=l+1, \ldots, n} | \log f_Y(Y_i) | \right) \), which is obtained in the same way, we conclude from (28) that
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in G} \frac{1}{n} \mathbb{E}_\tau \sum_{i=l+1}^{n} | (\log f_X f_Y(Z_{i}^{(1)})) \mathbb{1}_{\{A_i^c \cup (A_i')^c \}} | \lesssim k_1^* l_n \log n \to 0.
\] (30)

Moreover, given any \( \epsilon \in (0, (\alpha + 2d)/\alpha) \), set \( \epsilon' := \alpha \epsilon / (\alpha + 2d) \). Then by two applications of Hölder’s inequality,
\[
\frac{1}{n} \mathbb{E}_\tau \sum_{i=l+1}^{n} | (\log f_X f_Y(Z_{i}^{(1)})) \mathbb{1}_{\{Z_i^{(1)} \in W_n^c\}} | \leq \int_{W_n^c} f_X f_Y(z) | \log f_X f_Y(z) | dz \leq \nu p_n + \frac{\nu' \epsilon'}{\epsilon} \int_{W_n^c} f_X f_Y(z)^{1-\epsilon'} dz
\leq \nu p_n + \frac{\nu' \epsilon'}{\epsilon} p_n^{1-\epsilon} \left( \int_{W_n^c} f_X f_Y(z)^{2d/(\alpha + 2d)} dz \right)^{\epsilon'}
\leq \nu p_n + \frac{\nu' \epsilon'}{\epsilon} p_n^{1-\epsilon} \left[ \{1 + \max(1, 2^\alpha - 1)\mu\}^{2d/(\alpha + 2d)} \left( \int_{\mathbb{R}^d} \frac{1}{(1 + \|z\|^{\alpha})^{2d/\alpha}} dz \right)^{\alpha/(\alpha + 2d)} \right]^{\epsilon'} \lesssim p_n^{1-\epsilon}.
\] (31)

From (30) and (31), we find that
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in G} \max_{\tau \in \mathcal{J}_n} \frac{1}{n} \mathbb{E}_\tau \sum_{i=l+1}^{n} | (\log f_X f_Y(Z_{i}^{(1)})) \mathbb{1}_{\{(A_i^c) \cup (A_i')^c \}} | \to 0,
\] (32)

which takes care of the second term in (27).

For the third term in (27), since \( Z_{i}^{(1)} \) and \( \{Z_{i}^{(j)} : j \notin \{i, \tau(i), \tau^{-1}(i)\}\} \) are independent,
we have
\[
\mathbb{E}_\tau \left\{ \frac{1}{n} \sum_{i=l+1}^{n} \log f_X f_Y (Z_i^{(1)}) - \frac{n-l}{n} \{ H(X) + H(Y) \} \right\} \leq \text{Var}_\tau^{1/2} \left( \frac{1}{n} \sum_{i=l+1}^{n} \log f_X f_Y (Z_i^{(1)}) \right) \\
\leq \frac{3^{1/2}}{n^{1/2}} \text{Var}_\tau^{1/2} \log f_X f_Y (Z_n^{(1)}) \leq \frac{3^{1/2}}{n^{1/2}} \left[ \left\{ \mathbb{E} \log^2 f_X (X_1) \right\}^{1/2} + \left\{ \mathbb{E} \log^2 f_Y (Y_1) \right\}^{1/2} \right].
\]

By a very similar argument to that in (19), we deduce that
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in G_d \mathcal{X}, d \mathcal{Y}, \phi} \max_{\tau \in \bigcup_{l=0}^{1} S_l} |\mathbb{E}_{\tau} \left\{ \frac{1}{n} \sum_{i=l+1}^{n} \log f_X f_Y (Z_i^{(1)}) - \frac{n-l}{n} \{ H(X) + H(Y) \} \right\}| \to 0, \quad (33)
\]
which handles the third term in (27).

For the fourth term in (27), we simply observe that, by (19),
\[
\sup_{k \in \{k_0^*, \ldots, k_1^*\}} \sup_{f \in G_d \mathcal{X}, d \mathcal{Y}, \phi} \max_{\tau \in \bigcup_{l=0}^{1} S_l} \frac{1}{n} |H(X) + H(Y)| \to 0. \quad (34)
\]

Finally, we turn to the first term in (27). Recalling the definition of \( r_{z,f_X f_Y,\delta} \) in (4), we define the random variables
\[
N_{i,\delta} := \sum_{l+1 \leq j \leq n, j \neq i} \mathbb{1}_{\{ \| Z_j^{(1)} - Z_i^{(1)} \| \leq r_{Z_i^{(1)}, f_X f_Y, \delta} \}}.
\]

We study the bias and the variance of \( N_{i,\delta} \). For \( \delta \in (0, 2] \) and \( z \in \mathcal{W}_n \), we have that
\[
\mathbb{E}_\tau (N_{i,\delta} | Z_i^{(1)} = z) \geq (n - l - 3) \int_{B_x(r_{z,f_X f_Y,\delta})} f_X f_Y (w) \, dw \\
\geq (n - l - 3) \text{Var}_{x,f_X f_Y,\delta} \int_{B_x(r_{z,f_X f_Y,\delta})} f_X f_Y (z)(1 - c_n) \\
= \delta (1 - c_n) e^{\Psi(k)} \left( \frac{n - l - 3}{n - 1} \right). \quad (35)
\]

Similarly, also, for \( \delta \in (0, 2] \) and \( z \in \mathcal{W}_n \),
\[
\mathbb{E}_\tau (N_{i,\delta} | Z_i^{(1)} = z) \leq 2 + (n - l - 3) \int_{B_x(r_{z,f_X f_Y,\delta})} f_X f_Y (w) \, dw \\
\leq 2 + \delta (1 + c_n) e^{\Psi(k)} \left( \frac{n - l - 3}{n - 1} \right). \quad (36)
\]

33
Note that if \( j_2 \notin \{j_1, \tau(j_1), \tau^{-1}(j_1)\} \) then for \( \delta \in (0, 2) \) and \( z \in \mathcal{W}_n \),

\[
\text{Cov}_\tau\left( \mathbb{1}\{\| Z_{j_1}^{(1)} - z \| \leq r_{z,f_X f_Y, \delta} \}, \mathbb{1}\{\| Z_{j_2}^{(1)} - z \| \leq r_{z,f_X f_Y, \delta} \} | Z_i^{(1)} = z \right) = 0.
\]

Also, for \( j \notin \{i, \tau(i), \tau^{-1}(i)\} \) we have

\[
\text{Var}_\tau\left( \mathbb{1}\{\| Z_j^{(1)} - z \| \leq r_{z,f_X f_Y, \delta} \} | Z_i^{(1)} = z \right) \leq \int_{B_z(r_{z,f_X f_Y, \delta})} f_X f_Y(w) \, dw \leq \frac{\delta(1 + c_n) e^{\Psi(k)}}{n - 1}.
\]

When \( j \in \{i, \tau(i), \tau^{-1}(i)\} \) we simply bound the variance above by \( 1/4 \) so that, by Cauchy–Schwarz, when \( n - 1 \geq 2(1 + c_n e^{\Psi(k)}) \),

\[
\text{Var}_\tau(N_i, \delta | Z_i^{(1)} = z) \leq 3(n - l_n - 3) \frac{\delta(1 + c_n) e^{\Psi(k)}}{n - 1} + 1. \tag{37}
\]

Letting \( \epsilon_{n,k} := \max(k^{-1/2} \log n, c_n^{1/2}) \), there exists \( n_0 \in \mathbb{N} \), depending only on \( d_X, d_Y, \phi \) and \( k_0^* \), such that for \( n \geq n_0 \) and all \( k \in \{k_0^*, \ldots, k_1^*\} \), we have \( \epsilon_{n,k} \leq 1/2 \) and

\[
\min \left\{ (1 + \epsilon_{n,k})(1 - c_n) e^{\Psi(k)} \left( \frac{n - l_n - 3}{n - 1} \right) - k, k - 2 - (1 - \epsilon_{n,k})(1 + c_n) e^{\Psi(k)} \left( \frac{n - l_n - 3}{n - 1} \right) \right\} \geq \frac{k \epsilon_{n,k}}{2}.
\]

We deduce from (37) and (35) that for \( n \geq n_0 \),

\[
\mathbb{P}_\tau\left( \{\xi_i^{(1)} f_X f_Y(Z_i^{(1)}) - 1\} \mathbb{1}_{A_i} \geq \epsilon_{n,k}\right) = \mathbb{P}_\tau\left( A_i \cap \{\rho(k), i, (1) \geq r_{Z_i^{(1)}, f_X f_Y, 1 + \epsilon_{n,k}}\} \right)
\]

\[
\leq \mathbb{P}_\tau\left( N_{i,1 + \epsilon_{n,k}} \leq k, Z_i^{(1)} \in \mathcal{W}_n \right) = \int_{\mathcal{W}_n} f_X f_Y(z) \mathbb{P}_\tau\left( N_{i,1 + \epsilon_{n,k}} \leq k | Z_i^{(1)} = z \right) \, dz
\]

\[
\leq \int_{\mathcal{W}_n} f_X f_Y(z) \frac{\mathbb{V} \text{ar}_\tau\left( N_{i,1 + \epsilon_{n,k}} \mathbb{1}| Z_i^{(1)} = z \right) \}}{\mathbb{E}_\tau\left( N_{i,1 + \epsilon_{n,k}} \mathbb{1}| Z_i^{(1)} = z \right) - k}^2 \, dz
\]

\[
\leq 3(n - l_n - 3) \frac{(1 + \epsilon_{n,k})(1 + c_n) e^{\Psi(k)}}{n - 1} + 1 \frac{(1 + \epsilon_{n,k})(1 - c_n) e^{\Psi(k)} \left( \frac{n - l_n - 3}{n - 1} \right) - k}^2. \tag{38}
\]

Using very similar arguments, but using (36) in place of (35), we also have that for \( n \geq n_0 \),

\[
\mathbb{P}_\tau\left( \{\xi_i^{(1)} f_X f_Y(Z_i^{(1)}) - 1\} \mathbb{1}_{A_i} \leq -\epsilon_{n,k}\right) \leq \frac{3(n - l_n - 3)\left(1 - \epsilon_{n,k}\right)(1 + c_n) e^{\Psi(k)}}{n - 1} + 1 \left\{ k - 2 - (1 - \epsilon_{n,k})(1 + c_n) e^{\Psi(k)} \left( \frac{n - l_n - 3}{n - 1} \right) \right\}^2. \tag{39}
\]
Now, by Markov’s inequality, for \( k \geq 3, i \in \{l + 1, \ldots, n\} \), \( \tau \in S^l_n \) and \( \delta \in (0, 2] \),
\[
\mathbb{P}_\tau \left( \left\{ \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) \leq \delta \right\} \cap A_i \right) = \mathbb{P}_\tau \left( N_{i, \delta} \geq k, Z_i^{(1)} \in \mathcal{W}_n \right)
\leq \frac{n - l - 3}{k - 2} \int_{\mathcal{W}_n} f_X f_Y (z) \int_{B_z (r_z, f_X f_Y, t)} f_X f_Y (w) \, dw \, dz
\leq \frac{n - l - 3}{k - 2} (1 + c_n) \frac{\delta e^\psi(k)}{n - 1}.
\] (40)

Moreover, for any \( i \in \{l + 1, \ldots, n\} \), \( \tau \in S^l_n \) and \( t > 0 \), by two applications of Markov’s inequality,
\[
\mathbb{P}_\tau \left( \left\{ \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) \geq t \right\} \cap A_i \right) \leq \mathbb{P}_\tau \left( N_{i, t} \leq k, Z_i^{(1)} \in \mathcal{W}_n \right)
\leq \frac{n - l - 3}{n - l - k - 3} \int_{\mathcal{W}_n} f_X f_Y (z) \int_{B_z (r_z, f_X f_Y, t)} f_X f_Y (w) \, dw \, dz
\leq \frac{n - l - 3}{n - l - k - 3} \max \{1, 2^{\alpha - 1}\} \int_{\mathcal{W}_n} f_X f_Y (z) \mu + \|z\|^{\alpha/d} \, dz
\leq \frac{n - l - 3}{n - l - k - 3} \max \{1, 2^{\alpha - 1}\} 2 \mu t^{2^\alpha/d} V_\alpha/d \left( \frac{n - 1}{e^\psi(k)} \right)^{\alpha/d} t^{-\alpha/d}.
\] (41)

Writing \( s_n := \log^2 \left( (n/k) \log^{2d/\alpha} n \right) \), we deduce from (38), (39), (40) and (41) that for \( n \geq n_0 \),
\[
\mathbb{E}_\tau \left\{ \log^2 \left( \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) \right) 1_{A_i} \right\} = \int_0^\infty \mathbb{P}_\tau \left( \left\{ \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) \leq e^{-s^{1/2}} \right\} \cap A_i \right) \, ds
+ \log^2 (1 + \epsilon_{n,k}) \left( \int_{\log^2 (1 + \epsilon_{n,k})}^{s_n} + \int_{s_n}^\infty \right) \mathbb{P}_\tau \left( \left\{ \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) > e^{s^{1/2}} \right\} \cap A_i \right) \, ds
\leq \frac{n - l - 3}{k - 2} (1 + c_n) \frac{e^\psi(k)}{n - 1} \int_0^\infty e^{-s^{1/2}} \, ds + \log^2 (1 + \epsilon_{n,k})
+ s_n \frac{12(n - l - 3)(1 + c_n) e^\psi(k)}{n - 1} + 1
+ \frac{n - l - 3}{n - l - k - 3} \max \{1, 2^{\alpha - 1}\} 2 \mu t^{2^\alpha/d} V_\alpha/d \left( \frac{n - 1}{e^\psi(k)} \right)^{\alpha/d} \int_{s_n}^\infty e^{-s^{1/2} \alpha/d} \, ds.
\]

We conclude that
\[
\sup_{n \in \mathbb{N}} \sup_{k \in \{k_0, \ldots, k^*_1\}} \sup_{f \in \mathcal{G}_{d_X, d_Y, \phi}} \sup_{\tau \in \bigcup_{i=1}^{n} S^l_n} \max_{i \in \{l+1, \ldots, n\}} \mathbb{E}_\tau \left\{ \log^2 \left( \xi_i^{(1)} f_X f_Y (Z_i^{(1)}) \right) 1_{A_i} \right\} < \infty.
\] (42)
Finally, then, from (38), (39) and (42),
\[
\frac{1}{n} \sum_{i=l+1}^{n} \mathbb{E}_{\tau} \left| \log(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right| \leq \max_{i=l+1, \ldots, n} \mathbb{E}_{\tau} \left| \log(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right|
\leq 2\epsilon_{n,k} + \max_{i=l+1, \ldots, n} \left[ \mathbb{P}_{\tau} \left\{ \left| \log(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right| \geq 2\epsilon_{n,k} \right\} \mathbb{E}_{\tau} \left\{ \log^2(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right\} \right]^{1/2}
\leq 2\epsilon_{n,k} + \max_{i=l+1, \ldots, n} \left[ \mathbb{P}_{\tau} \left\{ \left| \xi_i f_Y(Z_{i}^{(1)}) \right| - 1 \mathbbm{1}_{A_i} \geq \epsilon_{n,k} \right\} \mathbb{E}_{\tau} \left\{ \log^2(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right\} \right]^{1/2},
\]
so
\[
\sup_{k \in \{k_0, \ldots, k_i\}} \sup_{f \in \mathcal{G}_{dX}, \phi \in \mathcal{U}_{l+1}^{n}} \max_{\tau \in \mathcal{I}_{l+1}^{n}} \frac{1}{n} \sum_{i=l+1}^{n} \mathbb{E}_{\tau} \left| \log(\xi_i f_Y(Z_{i}^{(1)})) \mathbbm{1}_{A_i} \right| \to 0. \tag{43}
\]
as \(n \to \infty\). The proof of claim (26) follows from (27), together with (32), (33), (34) and (43).

The final result therefore follows from (12), (13), (20), (21) and (26).

7.3 Proof from Section 5

Proof of Theorem 6. We partition \(X = (X_{(1)}^{T}, X_{(2)}^{T})^{T} \in \mathbb{R}^{(m+m) \times p}\) and, writing \(\eta^{(0)} := \epsilon/\sigma\), let \(\eta^{(b)} = ((\eta^{(b)}_{(1)})^{T}, (\eta^{(b)}_{(2)})^{T})^{T} \in \mathbb{R}^{m+m}\), for \(b = 0, \ldots, B\). Further, let \(\hat{\gamma} := (X_{(2)}^{T} X_{(2)})^{-1} X_{(2)}^{T} \eta^{(0)}_{(2)}, \hat{\gamma}^{(1)} := (X_{(2)}^{T} X_{(2)})^{-1} X_{(2)}^{T} \eta^{(1)}_{(2)}\) and \(\tilde{\sigma} := \hat{\sigma}_{(2)}/\sigma\). Now define the events
\[
A_{r_0, s_0} := \left\{ \max(\|\hat{\gamma}\|, \|\hat{\gamma}^{(1)}\|) \leq r_0, \tilde{\sigma} \in [s_0, 1/s_0], \tilde{\sigma}^{(1)} \in [s_0, 1/s_0] \right\}
\]
and \(A_0 := \{\lambda_{\min}(n^{-1} X^{T} X) > \frac{1}{2} \lambda_{\min}(\Sigma)\}\). Now
\[
\mathbb{P}(I_{n}^{(0)} \leq I_{n}^{(1)}) \leq \mathbb{P}(\{I_{n}^{(0)} \leq I_{n}^{(1)}\} \cap A_{r_0, s_0} \cap A_0) + \mathbb{P}(A^{c}_0) + \mathbb{P}(A_0 \cap A^{c}_{r_0, s_0}). \tag{44}
\]
For the first term in (44), define functions \(h, h^{(1)} : \mathbb{R}^{p} \to \mathbb{R}\) by
\[
h(b) := H(\eta_1 - X_{1}^{T} b) \quad \text{and} \quad h^{(1)}(b) := H(\eta^{(1)}_1 - X_{1}^{T} b).
\]
Now, for a density $g$ such that $f \in F_{\eta, \hat{\eta}, \gamma, \hat{\gamma}, s(1)}$ and $s, \hat{s} > 0$, we turn to the approach taken in Proposition 1 of Polyanskiy and Wu (2016). Write $a, \hat{a} \in A$ for the fifth
component of $\theta_1$, and for $x \in \mathbb{R}$ with $f_\eta(x) > 0$, let

$$r_{a_1}(x) := \frac{1}{8a_1(f_\eta(x))}.$$ 

Then, for $|y - x| \leq r_{a_1}(x)$ we have by Berrett, Samworth and Yuan (2017, Lemma 12) that

$$|f_\eta(y) - f_\eta(x)| \leq \frac{15}{7} f_\eta(x) a_1(f_\eta(x)) |y - x| \leq \frac{15}{56} f_\eta(x).$$

Hence

$$|\log f_\eta(y) - \log f_\eta(x)| \leq \frac{120}{41} a_1(f_\eta(x)) |y - x|.$$ 

When $|y - x| > r_{a_1}(x)$ we may simply write

$$|\log f_\eta(y) - \log f_\eta(x)| \leq 8\{|\log f_\eta(y)| + |\log f_\eta(x)|\} a_1(f_\eta(x)) |y - x|.$$ 

Combining these two equations we now have that, for any $x, y$ such that $f_\eta(x) > 0$,

$$|\log f_\eta(y) - \log f_\eta(x)| \leq 8\{1 + |\log f_\eta(y)| + |\log f_\eta(x)|\} a_1(f_\eta(x)) |y - x|.$$ 

By an application of the generalised Hölder inequality and Cauchy–Schwarz, we conclude that

$$\mathbb{E}\left|\log \frac{f_\eta(\eta_1 - X_1^T \gamma)}{f_\eta(\eta_1)}\right|$$

$$\leq 8\left\{\mathbb{E} a_1^2(f_\eta(\eta_1))\right\}^{1/2} \left\{\mathbb{E}\left\{(1 + |\log f_\eta(\eta_1 - X_1^T \gamma)| + |\log f_\eta(\eta_1)|)^2\right\}\right\}^{1/2} \left\{\mathbb{E}(|X_1^T \gamma|^4)\right\}^{1/4}$$

$$\leq 16\|\gamma\|^4\left\{\mathbb{E} a_1^2(f_\eta(\eta_1))\right\}^{1/2} \left\{\mathbb{E}\left\{1 + \log^2 f_\eta(\eta_1 - X_1^T \gamma) + \log^2 f_\eta(\eta_1)\right\}\right\}^{1/2} \left\{\mathbb{E}(|X_1|^4)\right\}^{1/4}. \quad (48)$$

We also obtain a similar bound on the quantity $\mathbb{E}\left|\log \frac{f_\eta^{-1}(\eta - X_1^T \gamma)}{f_\eta^{-1}(\eta)}\right|$ when $\|\gamma\| \leq r_0$. Moreover, for any random vectors $U, V$ with densities $f_U, f_V$ on $\mathbb{R}^d$ satisfying $H(U), H(V) \in \mathbb{R}$, and writing $\mathcal{U} := \{f_U > 0\}, \mathcal{V} := \{f_V > 0\}$, we have by the non-negativity of Kullback–Leibler divergence that

$$H(U) - H(V) = \int_V f_V \log f_V - \int_U f_U \log f_U - \int_U f_U \log \frac{f_U}{f_V} \leq \mathbb{E} \log \frac{f_V(V)}{f_U(U)}.$$
Combining this with the corresponding bound for $H(V) - H(U)$, we obtain that

$$|H(U) - H(V)| \leq \max \left\{ \mathbb{E} \left| \log \frac{f_U(U)}{f_V(V)} \right|, \mathbb{E} \left| \log \frac{f_V(V)}{f_U(U)} \right| \right\}. $$

Since $f_\eta, f_\eta^1 \in F_{1,\theta}$ when $\|\gamma\| \leq r_0$, we may apply (48), the second part of Berrett, Samworth and Yuan (2017, Proposition 9), (5), (6) and the fact that $\alpha_2 \geq 4$ to deduce that

$$\sup_{f \in F_{p+1,\omega}} \sup_{\gamma \in B^m_0(r_0)} \frac{|h(\gamma) - h(0)|}{\|\gamma\|} \leq \sup_{f \in F_{p+1,\omega}} \sup_{\gamma \in B^m_0(r_0)} \frac{1}{\|\gamma\|} \max \left\{ \mathbb{E} \left| \log \frac{f_\eta(\eta_1 - X_1^T \gamma)}{f_\eta(\eta)} \right|, \mathbb{E} \left| \log \frac{\hat{f}_\eta^1(\eta_1 - X_1^T \gamma)}{\hat{f}_\eta^1(\eta)} \right| \right\} < \infty. $$

(49)

Similarly,

$$\sup_{f \in F_{p+1,\omega}} \sup_{\gamma \in B^m_0(r_0)} \frac{|h^{(1)}(\gamma) - h^{(1)}(0)|}{\|\gamma\|} < \infty. $$

(50)

We now study the convergence of $\hat{\gamma}$ and $\hat{\gamma}^{(1)}$ to 0. By definition, the unique minimiser of the function

$$R(\beta) := \mathbb{E}\{(Y_1 - X_1^T \beta)^2\} = \mathbb{E}(\epsilon_1^2) - 2(\beta - \beta_0)^T \mathbb{E}(\epsilon_1 X_1) + (\beta - \beta_0)^T \Sigma (\beta - \beta_0)$$

is given by $\beta_0$, and $R(\beta_0) = \mathbb{E}(\epsilon_1^2)$. Now, for $\lambda > 0$,

$$R\left(\beta_0 + \lambda \mathbb{E}(\epsilon_1 X_1)\right) = \mathbb{E}(\epsilon_1^2) - 2\lambda \|\mathbb{E}(\epsilon_1 X_1)\|^2 + \lambda^2 \mathbb{E}(\epsilon_1 X_1)^T \Sigma \mathbb{E}(\epsilon_1 X_1).$$

If $\mathbb{E}(\epsilon_1 X_1) \neq 0$ then taking $\lambda = \frac{\|\mathbb{E}(\epsilon_1 X_1)\|^2}{\mathbb{E}(\epsilon_1 X_1)^T \Sigma \mathbb{E}(\epsilon_1 X_1)}$ we have $R\left(\beta_0 + \lambda \mathbb{E}(\epsilon_1 X_1)\right) < \mathbb{E}(\epsilon_1^2)$, a contradiction. Hence $\mathbb{E}(\epsilon_1 X_1) = 0$. Moreover,

$$\mathbb{E}\left\| \frac{1}{m} \sum_{i=m+1}^n X_i \eta_i \right\| \leq \frac{1}{m} \sum_{j=1}^p \mathbb{E} \left\| \sum_{i=m+1}^{\eta} X_{ij} \eta_i \right\| \leq \frac{1}{m} \sum_{j=1}^p \text{Var}^{1/2} \left( \sum_{i=m+1}^{\eta} X_{ij} \eta_i \right)$$

$$= \frac{1}{m^{1/2}} \sum_{j=1}^p \text{Var}^{1/2}(X_{ij} \eta_i) \leq \frac{2^{1/2} p}{n^{1/2}} \mathbb{E}(\eta_1^4)^{1/4} \max_{j=1,\ldots,p} \mathbb{E}(X_{1j})^{1/4}. $$

(51)
It follows that
\[
\mathbb{E}(\|\hat{\gamma}\| \mathbb{1}_{A_0}) = \mathbb{E}\left\{\| (X_{(2)}^T X_{(2)})^{-1} X_{(2)}^T \eta_{(2)}^{(0)} \| \mathbb{1}_{A_0} \right\} \leq \frac{2^{1/2} p \lambda_0 n \eta_1^{1/4}}{\lambda_0 n \eta_1^{1/4}} \max_{j=1,\ldots,p} \mathbb{E}(X_{1j}^4)^{1/4}. \tag{52}
\]

Similar arguments yield the same bound for \( \mathbb{E}(\|\hat{\gamma}^{(1)}\| \mathbb{1}_{A_0}) \). Hence, from (49), (50) and (52), we deduce that
\[
\limsup_{n \to \infty} n^{1/2} \sup_{f \in F_{p+1,\omega}} \mathbb{E}_f(\| R_2 \mathbb{1}_{A_{r_0, \eta_0} \cap A_0} \|) < \infty. \tag{53}
\]

We now bound \( \mathbb{P}(A_0^c) \). By the Hoffman–Wielandt inequality, we have that
\[
\{\lambda_{\min}(m^{-1} X_{(2)}^T X_{(2)} - \eta_{(0)}^{(2)} \| \mathbb{1}_{A_0})^2 \leq \| m^{-1} X_{(2)}^T X_{(2)} - \Sigma \|_F^2. \tag{54}
\]

Thus
\[
\mathbb{P}(A_0^c) \leq \mathbb{P}\left(\| m^{-1} X_{(2)}^T X_{(2)} - \Sigma \|_F \geq \frac{1}{2} \lambda_{\min}(\Sigma)\right) \leq \frac{4}{m \lambda_{\min}^2(\Sigma)} \sum_{j,l=1}^p \mathbb{V}(X_{1j} X_{1l}) \leq \frac{8 p^2}{n \lambda_{\min}^2(\Sigma)} \max_{j=1,\ldots,p} \mathbb{E}(X_{1j}^4). \tag{54}
\]

Finally, we bound \( \mathbb{P}(A_0 \cap A_{r_0, \eta_0}) \). By Markov’s inequality and (52),
\[
\mathbb{P}\left(\{\|\hat{\gamma}\| \geq r_0 \} \cap A_0\right) \leq \frac{1}{r_0} \mathbb{E}(\|\hat{\gamma}\| \mathbb{1}_{A_0}) \leq \frac{2^{1/2} p \lambda_0 n \eta_1^{1/4}}{r_0 \lambda_0 n \eta_1^{1/4}} \max_{j=1,\ldots,p} \mathbb{E}(X_{1j}^4)^{1/4}. \tag{55}
\]

The same bound also holds for \( \mathbb{P}(\{\|\hat{\gamma}^{(1)}\| \geq r_0 \} \cap A_0) \). Furthermore, writing \( P_{(2)} := X_{(2)}(X_{(2)}^T X_{(2)})^{-1} X_{(2)}^T, \) note that
\[
|S^2 - 1| = \left| \frac{1}{m} \| \eta_{(2)}^{(0)} \| ^2 - 1 - \frac{1}{m} \| P_{(2)} \eta_{(2)}^{(0)} \| ^2 \right| \leq \frac{1}{m} \left| \sum_{i=m+1}^n (\eta_i^2 - 1) \right| + \frac{1}{m} \eta_{(2)}^{(0)T} P_{(2)} \eta_{(2)}^{(0)}.
\]

40
so by Chebychev’s inequality, Markov’s inequality and (51), for any $\delta > 0$

$$
P(\{|\hat{s}^2 - 1| > \delta\} \cap A_0) 
\leq P \left( \left\{ \left| \frac{1}{m} \sum_{i=m+1}^{n} (\eta_i^2 - 1) \right| > \frac{\delta}{2} \right\} \cap A_0 \right) + P \left( \left\{ \left\| \frac{1}{m} X_T^{(0)} \eta_1^{(0)} \right\| > \left( \frac{\lambda_0 \delta}{2} \right)^{1/2} \right\} \cap A_0 \right) 
\leq 8 \frac{n \delta^2}{\eta_1^4} + \frac{2p}{\delta^{1/2} \lambda_0^{1/2}} \frac{\eta_1^4}{n^{1/2}} \max_{j=1,...,p} E(X_1^4)^{1/4}. \tag{56}
$$

The same bound holds for $P(\{|\hat{s}^{(1)}(1) - 1| > \delta\} \cap A_0)$. We conclude from Markov’s inequality, (44), (45), (47), (53), (54), (55) and (56) that

$$
sup_{\mathcal{B}_n \geq \mathcal{B}^*} \sup_{\mathcal{F}_{k_0,\ldots,k^*} \in \mathcal{F}^*_{1,p+1}: I(f) \geq b_n} \sup_{k \in \{k_0,\ldots,k^*\}} P_f(\tilde{I}_n \leq \tilde{C}^{(n),\mathcal{B}_n}) 
\leq \frac{1}{q(B_n^* + 1)} + \frac{1}{q(B_n^* + 1)} \sup_{k \in \{k_0,\ldots,k^*\}} \sup_{f \in \mathcal{F}_{1,p+1}: I(f) \geq b_n} P_f(\bar{\tilde{I}}_n^{(1)} \geq \tilde{I}_n^{(0)}) 
\leq \frac{1}{q(B_n^* + 1)} + \frac{1}{q(B_n^* + 1)} \sup_{k \in \{k_0,\ldots,k^*\}} \sup_{f \in \mathcal{F}_{1,p+1}: I(f) \geq b_n} \{P_f(\bar{\tilde{I}}_n^{(1)} \geq \tilde{I}_n^{(0)}) \cap A_{r,s,0} \cap A_0) 
+ P_f(A_0 \cap A_{r,s,0}^c) + P_f(A_0^c) \} 
\leq \frac{1}{q(B_n^* + 1)} + \frac{1}{q(B_n^* + 1)} \sup_{k \in \{k_0,\ldots,k^*\}} \sup_{f \in \mathcal{F}_{1,p+1}: I(f) \geq b_n} \left\{ \frac{1}{b_n} E_f(\left| R_1 + R_2 [I_{A_{r,s,0}}] \right|) 
+ P_f(A_0 \cap A_{r,s,0}^c) + P_f(A_0^c) \right\} \to 0,
$$
as required. \qed

**Acknowledgements:** Both authors are supported by an EPSRC Programme grant. The first author was supported by a PhD scholarship from the SIMS fund; the second author is supported by an EPSRC Fellowship and a grant from the Leverhulme Trust.

**References**

Albert, M., Bouret, Y., Fromont, M. and Reynaud-Bouret, P. (2015) Bootstrap and permutation tests of independence for point processes. *Ann. Statist.*, **43**, 2537–2564.
Bach, F. R. and Jordan, M. I. (2002) Kernel independent component analysis. *J. Mach. Learn. Res.*, **3**, 1–48.

Bergsma, W. and Dassios, A. (2014) A consistent test of independence based on a sign covariance related to Kendall’s tau. *Bernoulli*, **20**, 1006–1028.

Berrett, T. B., Grose, D. J. and Samworth, R. J. (2017) **IndepTest**: nonparametric independence tests based on entropy estimation. Available at https://cran.r-project.org/web/packages/IndepTest/index.html.

Berrett, T. B., Samworth, R. J. and Yuan, M. (2017) Efficient multivariate entropy estimation via $k$-nearest neighbour distances. https://arxiv.org/abs/1606.00304v3.

Biau, G. and Devroye, L. (2015) *Lectures on the Nearest Neighbor Method*. Springer, New York.

Comon, P. (1994) Independent component analysis, a new concept?. *Signal Process.*, **36**, 287–314.

Dalgaard, P. (2002) *Introductory Statistics with R*. Springer-Verlag, New York.

Dobson, A. J. (2002) *An Introduction to Generalized Linear Models*. Chapman & Hall, London.

Einmahl, J. H. J. and van Keilegom, I. (2008) Tests for independence in nonparametric regression. *Statistica Sinica*, **18**, 601–615.

Fan, J., Feng, Y. and Xia, L. (2017) A projection based conditional dependence measure with applications to high-dimensional undirected graphical models. Available at arXiv:1501.01617.

Fan, Y., Lafaye de Micheaux, P., Penev, S. and Salopek, D. (2017) Multivariate nonparametric test of independence. *J. Multivariate Anal.*, **153**, 189–210.

Gibbs, A. L. and Su, F. E. (2002) On choosing and bounding probability metrics. *Int. Statist. Review*, **70**, 419–435.

Gretton A., Bousquet O., Smola A. and Schölkopf B. (2005) Measuring Statistical Dependence with Hilbert-Schmidt Norms. *Algorithmic Learning Theory*, 63–77.
Gretton, A. and Györfi, L. (2010) Consistent nonparametric tests of independence. *J. Mach. Learn. Res.*, 11, 1391–1423.

Heller, R., Heller, Y., Kaufman, S., Brill, B. and Gorfine, M. (2016) Consistent distribution-free K-sample and independence tests for univariate random variables. *J. Mach. Learn. Res.*, 17, 1–54.

Hoeffding, W. (1948) A non-parametric test of independence. *Ann. Math. Statist.*, 19, 546–557.

Hofert, M., Kojadinovic, I., Mächler, M. and Yan, J. (2017) *copula*: Multivariate Dependence with Copulas. *R Package version 0.999-18*. Available from https://cran.r-project.org/web/packages/copula/index.html.

Jitkrittum, W., Szabó, Z. and Gretton, A. (2016) An adaptive test of independence with analytic kernel embeddings. Available at arXiv:1610.04782.

Joe, H. (1989) Relative entropy measures of multivariate dependence. *J. Amer. Statist. Assoc.*, 84, 157–164.

Josse, J. and Holmes, S. (2016) Measuring multivariate association and beyond. *Statist. Surveys*, 10, 132–167.

Kojadinovic, I. and Holmes, M. (2009) Tests of independence among continuous random vectors based on Cramér–von Mises functionals of the empirical copula process. *J. Multivariate Anal.*, 100, 1137–1154.

Kozachenko, L. F. and Leonenko, N. N. (1987) Sample estimate of the entropy of a random vector. *Probl. Inform. Transm.*, 23, 95–101.

Lauritzen, S. L. (1996) *Graphical Models*. Oxford University Press, Oxford.

Mari, D. D. and Kotz, S. (2001) *Correlation and Dependence*. Imperial College Press, London.

Miller, E. G. and Fisher, J. W. (2003) ICA using spacings estimates of entropy. *J. Mach. Learn. Res.*, 4, 1271–1295.

Müller, U. U., Schick, A. and Wefelmeyer, W. (2012) Estimating the error distribution function in semiparametric additive regression models. *J. Stat. Plan. Inference*, 142, 552–566.
Neumeyer, N. (2009) Testing independence in nonparametric regression. *J. Multivariate Anal.*, **100**, 1551–1566.

Neumeyer, N. and Van Keilegom, I. (2010) Estimating the error distribution in nonparametric multiple regression with applications to model testing. *J. Multivariate Anal.*, **101**, 1067–1078.

Nguyen, D. and Eisenstein, J. (2017) A kernel independence test for geographical language variation. *Comput. Ling.*, to appear.

Pearl, J. (2009) *Causality*. Cambridge University Press, Cambridge.

Pearson, K. (1920) Notes on the history of correlation. *Biometrika*, **13**, 25–45.

Peixoto, J. L. (1990) A property of well-formulated polynomial regression models. *The American Statistician*, **44**, 26–30.

Pfister, N., Bühlmann, P., Schölkopf, B. and Peters, J. (2017) Kernel-based tests for joint independence. *J. Roy. Statist. Soc., Ser. B*, to appear.

Pfister, N. and Peters, J. (2017) dHSIC: Independence Testing via Hilbert Schmidt Independence Criterion. *R Package version 2.0*. Available at [https://cran.r-project.org/web/packages/dHSIC/index.html](https://cran.r-project.org/web/packages/dHSIC/index.html).

Polyanskiy, Y. and Wu, Y. (2016) Wasserstein continuity of entropy and outer bounds for interference channels. *IEEE Trans. Inf. Theory*, **62**, 3992–4002.

Rizzo, M. L. and Szekely, G. J. (2017) *energy: E-Statistics: Multivariate Inference via the Energy of Data*. *R Package version 1.7-2*. Available from [https://cran.r-project.org/web/packages/energy/index.html](https://cran.r-project.org/web/packages/energy/index.html).

Samworth, R. J. and Yuan, M. (2012) Independent component analysis via nonparametric maximum likelihood estimation. *Ann. Statist.*, **40**, 2973–3002.

Schweizer, B. and Wolff, E. F. (1981) On nonparametric measures of dependence for random variables. *Ann. Statist.*, **9**, 879–885.

Sejdinovic, D., Sriperumbudur, B., Gretton, A. and Fukumizu, K. (2013) Equivalence of distance-based and RKHS-based statistics in hypothesis testing. *Ann. Statist.*, **41**, 2263–2291.
Sen, A. and Sen, B. (2014) Testing independence and goodness-of-fit in linear models. *Biometrika*, **101**, 927–942.

Shah, R. D. and Bühlmann, P. (2017) Goodness of fit tests for high-dimensional linear models. *J. Roy. Statist. Soc., Ser. B*, to appear.

Song, L., Smola, A., Gretton, A., Bedo, J. and Borgwardt, K. (2012) Feature selection via dependence maximization. *J. Mach. Learn. Res.*, **13**, 1393–1434.

Steuer, R., Kurths, J., Daub, C. O., Weise, J. and Selbig, J. (2002) The mutual information: detecting and evaluating dependencies between variables. *Bioinformatics*, **18**, 231–240.

Stigler, S. M. (1989) Francis Galton’s account of the invention of correlation. *Stat. Sci.*, **4**, 73–86.

Su, L. and White, H. (2008) A nonparametric Hellinger metric test for conditional independence. *Econometric Theory*, **24**, 829–864.

Székely, G. J., Rizzo, M. L. and Bakirov, N. K. (2007) Measuring and testing dependence by correlation of distances. *Ann. Statist.*, **35**, 2769–2794.

Székely, G. J. and Rizzo, M. L. (2013) The distance correlation $t$-test of independence in high dimension. *J. Multivariate Anal.*, **117**, 193–213.

Torkkola, K. (2003) Feature extraction by non-parametric mutual information maximization. *J. Mach. Learn. Res.*, **3**, 1415–1438.

Vinh, N. X., Epps, J. and Bailey, J. (2010) Information theoretic measures for clusterings comparison: variants, properties, normalisation and correction for chance. *J. Mach. Learn. Res.*, **11**, 2837–2854.

Weihs, L., Drton, M. and Leung, D. (2016) Efficient computation of the Bergsma–Dassios sign covariance. *Comput. Stat.*, **31**, 315–328.

Weihs, L., Drton, M. and Meinshausen, N. (2017) Symmetric rank covariances: a generalised framework for nonparametric measures of dependence. https://arxiv.org/abs/1708.05653.

Wu, E. H. C., Yu, P. L. H. and Li, W. K. (2009) A smoothed bootstrap test for independence based on mutual information. *Comput. Stat. Data Anal.*, **53**, 2524–2536.
Yao, S., Zhang, X. and Shao, X. (2017) Testing mutual independence in high dimension via
distance covariance. *J. Roy. Statist. Soc., Set. B*, to appear.

Zhang, K., Peters, J., Janzing, D. and Schölkopf, B. (2011) Kernel-based conditional inde-
pendence test and application in causal discovery. https://arxiv.org/abs/1202.3775.

Zhang, Q., Filippi, S., Gretton, A. and Sejdinovic, D. (2017) Large-scale kernel methods for
independence testing. *Stat. Comput.*, 27, 1–18.