

The Hardness of Conditional Independence Testing and the Generalised Covariance Measure

Rajen D. Shah*

University of Cambridge, UK
r.shah@statslab.cam.ac.uk

Jonas Peters†

University of Copenhagen, Denmark
jonas.peters@math.ku.dk

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Abstract

It is a common saying that testing for conditional independence, i.e., testing whether X is independent of Y , given Z , is a hard statistical problem if Z is a continuous random variable. In this paper, we prove that conditional independence is indeed a particularly difficult hypothesis to test for. Statistical tests are required to have a size that is smaller than a predefined significance level, and different tests usually have power against a different class of alternatives. We prove that a valid test for conditional independence does not have power against *any* alternative.

Given the non-existence of a uniformly valid conditional independence test, we argue that tests must be designed so their suitability for a particular problem setting may be judged easily. To address this need, we propose in the case where X and Y are univariate to nonlinearly regress X on Z , and Y on Z and then compute a test statistic based on the sample covariance between the residuals, which we call the generalised covariance measure (GCM). We prove that validity of this form of test relies almost entirely on the weak requirement that the regression procedures are able to estimate the conditional means X given Z , and Y given Z , at a slow rate. We extend the methodology to handle settings where X and Y may be multivariate or even high-dimensional. While our general procedure can be tailored to the setting at hand by combining it with any regression technique, we develop the theoretical guarantees for kernel ridge regression. A simulation study shows that the test based on GCM is competitive with state of the art conditional independence tests. Code will be available as an R package.

1 Introduction

Conditional independences lie at the heart of several fundamental concepts such as sufficiency [22] and ancillarity [23, 24]; see also Jensen and Sørensen [29]. Dawid [17] states that “many results and theorems concerning these concepts are just applications of some simple general properties of conditional independence”. During the last few decades, conditional independence relations have played an increasingly important role in computational statistics, too, since they are the building blocks of graphical models [36, 33, 41].

Estimating conditional independence graphs has been of great interest in high-dimensional statistics, particularly in biomedical applications [e.g. 39, 19]. To estimate the conditional

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independence graph corresponding to a random vector $X \in \mathbb{R}^d$, edges may be placed between vertices corresponding to X_j and X_k if a test for whether X_j is conditionally independent of X_k given all other variables indicates rejection.

Conditional independence tests also play a key role in causal inference. Constraint-based or independence-based methods [41, 52, 43] apply a series of conditional independence tests in order to learn causal structure from observational data. The recently introduced invariant prediction methodology [42, 27] aims to estimate for a specified target variable Y , the set of causal variables among potential covariates X_1, \dots, d . Given data from different environments labelled by a variable E , the method involves testing for each subset $S \subseteq \{1, \dots, d\}$, the null hypothesis that the environment E is conditionally independent of Y , given X_S .

Given the importance of conditional independence tests in modern statistics, there has been great deal of work devoted to developing conditional independence tests; we review some important examples of tests in Section 1.3. However one issue that conditional independence tests appear to suffer from is that they can fail to control the type I error in finite samples, which can have important consequences in downstream analyses.

In the first part of this paper, we prove this failure of type I error control is in fact unavoidable: conditional independence is not a testable hypotheses. To fix ideas, consider n i.i.d. observations corresponding to a triple of random variables (X, Y, Z) where it is desired to test whether X is conditional independent of Y given Z . We show that provided the joint distribution of $(X, Y, Z) \in \mathbb{R}^{d_X + d_Y + d_Z}$ is absolutely continuous with respect to Lebesgue measure, any test based on the data whose size is less than a pre-specified level α , has no power; more precisely, there is no alternative, for which the test has power more than α . This result is perhaps surprising as it is in stark contrast to unconditional independence testing, for which permutation tests allow for the correct calibration of any hypothesis test. Our result implies that in order to perform conditional independence testing, some domain knowledge is required in order to select an appropriate conditional independence test for the particular problem setting at hand. This would appear to be challenging in practice, as the validity of conditional independence tests typically rests on properties of the entire joint distribution of the data, which may be hard to model.

Our second main contribution aims to alleviate this issue by providing a family of conditional independence tests whose validity relies on estimating the conditional expectations $\mathbb{E}(X|Z = z)$ and $\mathbb{E}(Y|Z = z)$ via regressions, in the setting where $d_X = d_Y = 1$. These need to be estimated sufficiently well using the data such that the product of mean squared prediction errors from the two regressions is $o(n^{-1})$. This is a relatively mild requirement that allows for settings where the conditional expectations are as general as Lipschitz functions, for example, and also encompasses settings where Z is high-dimensional but the conditional expectations have more structure.

Our test statistic, which we call the *generalised covariance measure* (GCM) is based on a suitably normalised version of the empirical covariance between the residual vectors from the regressions. The practitioner is free to choose the regression methods that appear most suitable for the problem of interest. Although domain knowledge is still required to make an appropriate choice, selection of regression methods is a problem statisticians are more familiar with. We also extend the GCM to handle settings where X and Y are potentially high-dimensional, though in this case our proof of the validity of the test additionally requires the errors $X_j - \mathbb{E}(X_j|Z)$ and $Y_k - \mathbb{E}(Y_k|Z)$ to obey certain moment restrictions for $j = 1, \dots, d_X$ and $k = 1, \dots, d_Y$ and slightly faster rates of convergence for the prediction errors.

As an example application of our results on the GCM, we consider the case where the regressions are performed using kernel ridge regression, and show that provided the conditional expectations are contained in a reproducing kernel Hilbert space, our test statistic has a tractable

limit distribution.

The rest of the paper is organised as follows. In Sections 1.1 and 1.2, we first formalise the notion of conditional independence and relevant concepts related to statistical hypothesis testing. In Section 1.3 we review some popular conditional independence tests, after which we set out some notation used throughout the paper. In Section 2 we present our main result on the hardness of conditional independence testing. We introduce the generalised covariance measure in Section 3 first treating the univariate case with $d_X = d_Y = 1$ before extending ideas to the potentially high-dimensional case. In Section 4 we apply the theory and methodology of the previous section to study that particular example of generalised covariance measures based on kernel ridge regression. We present numerical experiments in Section 5 and conclude with a discussion in Section 6. All proofs are deferred to the appendix and supplementary material.

1.1 Conditional Independence

Let us consider three random vectors X , Y and Z taking values in \mathbb{R}^{d_X} , \mathbb{R}^{d_Y} and \mathbb{R}^{d_Z} , respectively, and let us assume, for now that their joint distribution is absolutely continuous with respect to Lebesgue measure with density p . For our deliberations only the continuity in Z is necessary, see Remark 4. We say that X is conditionally independent of Y given Z and write

$$X \perp\!\!\!\perp Y | Z$$

if for all x, y, z with $p(z) > 0$, we have $p(x, y | z) = p(x | z)p(y | z)$, see, e.g., Dawid [17]. Here and below, statements involving densities should be understood to hold (Lebesgue) almost everywhere. We now discuss an equivalent formulation of conditional independence that has given rise to several hypothesis tests, including the generalised covariance measure proposed in this paper. Let therefore $L_{X,Z}^2$ denote the space of all functions $f : \mathbb{R}^{d_X} \times \mathbb{R}^{d_Z} \rightarrow \mathbb{R}$ such that $\mathbb{E}f(X, Z)^2 < \infty$ and define $L_{Y,Z}^2$ analogously. Daudin [16] proves that X and Y are conditionally independent given Z if and only if

$$\mathbb{E}f(X, Z)g(Y, Z) = 0 \tag{1}$$

for all functions $f \in L_{X,Z}^2$ and $g \in L_{Y,Z}^2$ such that $\mathbb{E}[f(X, Z)|Z] = 0$ and $\mathbb{E}[g(Y, Z)|Z] = 0$, respectively.

This may be viewed as an extension of the fact that for one-dimensional X and Y , the partial correlation coefficient $\rho_{X,Y|Z}$ (the correlation between residuals of linear regressions of X on Z and Y on Z) is 0 if and only if $X \perp\!\!\!\perp Y | Z$ in the case where (X, Y, Z) are jointly Gaussian.

1.2 Statistical Hypothesis Testing

We now introduce some notation and relevant concepts related to statistical hypothesis testing. In order to deal with composite null hypotheses where the probabilities of the event $\{\psi_n = 1\}$ must be controlled under a variety of different distributions for the data to which ψ_n is applied, we introduce the following notation. We will write $\mathbb{E}_P(\cdot)$ for expectations of random variables whose distribution is determined by P , and similarly $\mathbb{P}_P(\cdot) = \mathbb{E}_P \mathbb{1}_{\{\cdot\}}$.

Let \mathcal{P} be a potentially composite null hypothesis consisting of a collection of distributions for (X, Y, Z) . For $i = 1, 2, \dots$ let $(x_i, y_i, z_i) \in \mathbb{R}^{d_X+d_Y+d_Z}$ be i.i.d. copies of (X, Y, Z) and let $\mathbf{X}^{(n)} \in \mathbb{R}^{d_X \cdot n}$, $\mathbf{Y}^{(n)} \in \mathbb{R}^{d_Y \cdot n}$ and $\mathbf{Z}^{(n)} \in \mathbb{R}^{d_Z \cdot n}$ be matrices with i th rows x_i , y_i and z_i respectively. Let ψ_n be a potentially randomised test that can be applied to the data $(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$; formally,

$$\psi_n : \mathbb{R}^{(d_X+d_Y+d_Z) \cdot n} \times [0, 1] \rightarrow \{0, 1\}$$

is a measurable function whose last argument is reserved for a random variable $U \sim U[0, 1]$ independent of the data and that is responsible for the randomness of the test.

Given a sequence of tests $(\psi_n)_{n=1}^\infty$, the following validity properties will be of interest; note the particular names given to these properties differ in literature. Given a level $\alpha \in (0, 1)$ and null hypothesis \mathcal{P} , we say that the test ψ_n has

$$\text{valid level at sample size } n \text{ if } \sup_{P \in \mathcal{P}} \mathbb{P}_P(\psi_n = 1) \leq \alpha,$$

where the left-hand side is the *size* of the test; the sequence $(\psi_n)_{n=1}^\infty$ has

$$\text{uniformly asymptotic level if } \limsup_{n \rightarrow \infty} \sup_{P \in \mathcal{P}} \mathbb{P}_P(\psi_n = 1) \leq \alpha,$$

$$\text{pointwise asymptotic level if } \sup_{P \in \mathcal{P}} \limsup_{n \rightarrow \infty} \mathbb{P}_P(\psi_n = 1) \leq \alpha.$$

In practice, we would like a test to have at least uniformly asymptotic level. Otherwise, even for an arbitrarily large sample size n , there can exist null distributions for which the size exceeds the nominal level by some fixed amount.

Given a sequence of tests $(\psi_n)_{n=1}^\infty$ each with valid level $\alpha \in (0, 1)$ and alternative hypothesis \mathcal{Q} , it is desirable for the power to be large uniformly over \mathcal{Q} , and to have $\inf_{Q \in \mathcal{Q}} \mathbb{P}_Q(\psi_n = 1) \rightarrow 1$. In standard parametric settings, we can certainly achieve this for any fixed alternative hypothesis and indeed have uniform power against a sequence of \sqrt{n} alternatives. Nonparametric problems are much harder and when \mathcal{Q} contains all distributions outside a fixed total variation (TV) neighbourhood of \mathcal{P} , we have

$$\liminf_{n \rightarrow \infty} \inf_{Q \in \mathcal{Q}} \mathbb{P}_Q(\psi_n = 1) < 1,$$

[37, 3]. To achieve power tending to 1, we need to restrict \mathcal{Q} by imposing certain smoothness conditions for example [2].

A class of even harder hypothesis testing problems may be defined as those where no test with valid level achieves power at any alternative, so $\inf_{Q \in \mathcal{Q}} \mathbb{P}_Q(\psi_n = 1) \leq \alpha$. In other words, for all n , tests ψ_n and alternative distributions $Q \in \mathcal{Q}$, we have

$$\mathbb{P}_Q(\psi_n = 1) \leq \sup_{P \in \mathcal{P}} \mathbb{P}_P(\psi_n = 1).$$

The hypothesis testing problem defined by the pair $(\mathcal{P}, \mathcal{Q})$ is then said to be *untestable* [20]. In order to have power at even a single alternative, we need to restrict the null \mathcal{P} in some way. One of the main results of this paper is that conditional independence is untestable.

1.3 Related Work

Our hardness result for conditional independence contributes to an important literature on impossibility results in statistics and econometrics starting with the work of Bahadur and Savage [1] which shows that there is no non-trivial test for whether a distribution has mean zero. Canay et al. [11] shows that certain problems arising in the context of identification of some nonparametric models are not testable. In these examples, the null hypothesis is dense with respect to the TV metric in the alternative hypothesis, a property which implies untestability [49]. Interestingly, our Proposition 5 shows that conditional independence testing is qualitatively different in that distributions in the alternative are in fact well-separated from the null. It has been suggested for some time that conditional independence testing is a hard problem [see, e.g., 4, and several talks given by Bernhard Schölkopf]. To the best of our knowledge the conjecture

that conditional independence is not testable (cf. Corollary 3 with $M = \infty$) is due to Arthur Gretton.

We now briefly review several tests for conditional independence that bear some relation to our proposal here.

Extensions of partial correlation Ramsey [44], for example, suggests regressing X on Z and Y on Z and then testing for independence between the residuals. Fan et al. [21] consider this sort of approach in the setting where Z is potentially high-dimensional and under the null hypothesis of $X \perp\!\!\!\perp Y|Z$, $X = Z^T \beta_X + \varepsilon_X$, $Y = Z^T \beta_Y + \varepsilon_Y$ with $\varepsilon_X \perp\!\!\!\perp Z$ and $\varepsilon_Y \perp\!\!\!\perp Z$. They derive the asymptotic distribution of a test statistic based on distance covariance under certain additional conditions on the distributions of ε_X and ε_Y , and the ability to estimate β_X and β_Y . The following simple example however indicates where such methods can fail.

Example 1. Define N_X, N_Y and Z to be i.i.d. random variables with distribution $\mathcal{N}(0, 1)$ and define $X := Z \cdot N_X$, $Y := Z \cdot N_Y$. This implies $X \perp\!\!\!\perp Y|Z$. Since $\mathbb{E}[X|Z] = \mathbb{E}[Y|Z] = 0$, the (population) residuals equal $R_1 := Z \cdot N_X$ and $R_2 := Z \cdot N_Y$; they are uncorrelated but not independent since, e.g., $\text{cov}(R_1^2, R_2^2) \neq 0$. Any independence test that has power against this alternative will tend to reject the null hypothesis with large probability.

Kernel-based conditional independence tests Recently, conditional independence tests have been proposed that are based on reproducing kernel Hilbert spaces. The Hilbert-Schmidt independence criterion (HSIC) equals the square of the Hilbert-Schmidt norm of the cross-covariance operator, and is used in unconditional independence testing [26]. Fukumizu et al. [25] have extended these ideas to the conditional cross-covariance operator. The distribution of the test statistic under the null hypothesis is unknown, however, and has to be approximated by a resampling scheme. For continuous variables Z , this requires clustering of the values of Z and permuting X and Y values within the same cluster component. Zhang et al. [55] construct the kernel conditional independence (KCI) test by kernelizing a variation of Daudin's result (1). The authors state that their test yields pointwise asymptotic level control.

Estimation of expected conditional covariance Though typically not thought of as conditional independence tests, there are several approaches to estimating the expected conditional covariance functional $\mathbb{E}\text{cov}(X, Y|Z)$ in the semiparametric statistics literature [46, 15, 40]. From (1) we see these may be used as conditional independence tests and indeed the GCM test we propose falls under this category. We delay further discussion of such methods to Section 3.1.2.

1.4 Notation

We now introduce some notation used throughout the paper. If $(V_{P,n})_{n \in \mathbb{N}, P \in \mathcal{P}}$ is a family of sequences of random variables whose distributions are determined by $P \in \mathcal{P}$, we use $V_{P,n} = o_{\mathcal{P}}(1)$ and $V_{P,n} = O_{\mathcal{P}}(1)$ to mean respectively that for all $\epsilon > 0$,

$$\sup_{P \in \mathcal{P}} \mathbb{P}_P(|V_{P,n}| > \epsilon) \rightarrow 0, \quad \text{and} \\ \text{there exists } M > 0 \text{ such that } \sup_{P \in \mathcal{P}} \sup_{n \in \mathbb{N}} \mathbb{P}_P(|V_{P,n}| > M) < \epsilon.$$

If $(W_{P,n})_{n \in \mathbb{N}, P \in \mathcal{P}}$ is a further family of sequences of random variables, $V_{P,n} = o_{\mathcal{P}}(W_{P,n})$ and $V_{P,n} = O_{\mathcal{P}}(W_{P,n})$ mean $V_{P,n} = W_{P,n} R_{P,n}$ and respectively that $R_{P,n} = o_{\mathcal{P}}(1)$ and $R_{P,n} = O_{\mathcal{P}}(1)$. If \mathbf{A} is a $c \times d$ matrix, then \mathbf{A}_j denotes the j th column of \mathbf{A} , $j \in \{1, \dots, d\}$.

2 No-free-lunch in Conditional Independence Testing

In this section we show that, under certain conditions, no non-trivial test for conditional independence with valid level exists. To state our result, we introduce the following subsets of \mathcal{E}_0 defined to be the set of all distributions for (X, Y, Z) absolutely continuous with respect to Lebesgue measure.

Let $\mathcal{P}_0 \subset \mathcal{E}_0$ be the subset of distributions under which $X \perp\!\!\!\perp Y|Z$. Further, for any $M \in (0, \infty]$, let $\mathcal{E}_{0,M} \subseteq \mathcal{E}_0$ be the subset of all distributions with support contained strictly within an ℓ_∞ ball of radius M . Here we take $\mathcal{E}_{0,\infty} = \mathcal{E}_0$. We also define $\mathcal{Q}_0 = \mathcal{E}_0 \setminus \mathcal{P}_0$ and set $\mathcal{P}_{0,M} = \mathcal{E}_{0,M} \cap \mathcal{P}_0$, and $\mathcal{Q}_{0,M} = \mathcal{E}_{0,M} \cap \mathcal{Q}_0$. Consider the setup of Section 1.2 with null hypothesis $\mathcal{P} = \mathcal{P}_{0,M}$. Our first result shows that with this null hypothesis, any test ψ_n with valid level at sample size n has no power against any alternative.

Theorem 2 (No-free-lunch). *Given any $n \in \mathbb{N}$, $\alpha \in (0, 1)$, $M \in (0, \infty]$, and any potentially randomised test ψ_n that has valid level α for the null hypothesis $\mathcal{P}_{0,M}$, we have that $\mathbb{P}_Q(\psi_n = 1) \leq \alpha$ for all $Q \in \mathcal{Q}_{0,M}$. Thus ψ_n cannot have power against any alternative.*

A proof is given in the appendix. Note that taking M to be finite ensures all the random vectors (x_i, y_i, z_i) are bounded. Thus, for example, averages will converge in distribution to Gaussian limits uniformly over $\mathcal{P}_{0,M}$; however, as the result shows, this does not help in the construction of a non-trivial test for conditional independence. An immediate corollary to Theorem 2 is that there is no non-trivial test for conditional independence with uniformly asymptotic level.

Corollary 3. *For all $M \in (0, \infty]$ and for any sequence $(\psi_n)_{n=1}^\infty$ of tests we have*

$$\sup_{Q \in \mathcal{Q}_{0,M}} \limsup_{n \rightarrow \infty} \mathbb{P}_Q(\psi_n = 1) \leq \sup_{P \in \mathcal{P}_{0,M}} \limsup_{n \rightarrow \infty} \mathbb{P}_P(\psi_n = 1).$$

This result is in stark contrast to unconditional independence testing, where a permutation test can always be used to control the size of any testing procedure. As a consequence, there exist tests with valid level at sample size n and non-trivial power. For example, Hoeffding [28] introduces a rank-based test in the case of univariate random variables and proves that it maintains uniformly asymptotic level and has asymptotic power against each fixed alternative. For the multivariate case, Berrett and Samworth [5] considers a test based on mutual information and proves level guarantees, as well as uniform power results against a wide class of alternatives. Thus while independence testing remains a hard problem in that it is only possible to have uniform power against certain subsets of alternatives, this is different to conditional independence testing where we can only hope to control the size uniformly over certain subsets of the null hypothesis.

Remark 4. *Inspection of the proof shows that Theorem 2 also holds in the case where the variables X and Y have marginal distributions that are absolutely continuous with respect to counting measure, for example. Theorem 2 therefore contains an impossibility result for testing the equality of two conditional distributions (by taking Y to be an indicator specifying the distribution). The continuity of Z , however, is necessary. If Z only takes values in $\{1, 2\}$, for example, one can reduce the problem of conditional independence testing to unconditional independence testing by combining the tests for $X \perp\!\!\!\perp Y | Z = 1$ and $X \perp\!\!\!\perp Y | Z = 2$.*

The null hypothesis being dense with respect to TV distance among the alternative hypothesis is a sufficient condition for the problem to be untestable [49]. Proposition 5, proved in the supplementary material, illustrates that this is not the case here: at least for $M \in (0, \infty)$, there exists an alternative, for which there is no distribution from the null that is arbitrarily close.

Proposition 5. For $P, Q \in \mathcal{E}_0$, the total variation distance is given by

$$\|P - Q\|_{TV} := \sup_{A \in \mathcal{B}} |\mathbb{P}_P((X, Y, Z) \in A) - \mathbb{P}_Q((X, Y, Z) \in A)|,$$

where \mathcal{B} is the Borel σ -algebra on $\mathbb{R}^{d_X+d_Y+d_Z}$. For each $M \in (0, \infty)$, there exists $Q \in \mathcal{Q}_{0,M}$ satisfying

$$\inf_{P \in \mathcal{P}_{0,M}} \|P - Q\|_{TV} \geq 1/24.$$

In Proposition 16 in the appendix, we also show that the null and alternative hypotheses are well-separated in the sense of KL divergence. On the other hand, it is known that if a problem is untestable, the convex closure of the null must contain the alternative [35, 6, Theorem 5 and Corollary 1, respectively]. The problem of conditional independence testing therefore has the interesting property of the null being separated from the alternative, but its convex hull is TV-dense in the alternative.

A practical implication of the negative result of Theorem 2 is that domain knowledge is needed to select a conditional independence test appropriate for the data at hand. However guessing the form of the entire joint distribution in order to apply a test with the appropriate type I error control seems challenging. In Section 3 we introduce a form of test that instead relies on selecting regression methods that have sufficiently low prediction error when regressing $\mathbf{Y}^{(n)}$ and $\mathbf{X}^{(n)}$ on $\mathbf{Z}^{(n)}$, thereby converting the problem of finding an appropriate test to the more familiar task of prediction. Before discussing this methodology, we first sketch some of the main ideas of the proof of Theorem 2 below.

2.1 Proof ideas of Theorem 2

Consider the case where $d_X = d_Y = d_Z = 1$ and where the test is required to be non-randomised. First suppose that for $Q \in \mathcal{Q}_{0,M}$, we have a test with rejection region $R := \psi_n^{-1}(1) \subseteq \mathbb{R}^{3 \cdot n}$ such that $\mathbb{P}_Q((\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)}) \in R) > \alpha$. Let us suppose for now that R has the particularly simple form of a finite union of boxes. Our argument now proceeds by showing that one can construct a distribution $P \in \mathcal{P}_{0,M}$ from the null such that there is a coupling of P and Q where n -samples from each distribution are ϵ close in ℓ_∞ -norm. For a sufficiently small ϵ , we will have $\mathbb{P}_P((\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)}) \in R) > \alpha$ as well, giving the result.

Figure 1 sketches the main components in our construction of P , which is laid out formally in Lemmas 13 and 14 in the appendix. The key idea is as follows. Given $(X, Y, Z) \sim P$, we consider a binary expansion of (X, Y, Z) , which we truncate at some point to obtain $(\hat{X}, \hat{Y}, \hat{Z})$. We then concatenate the digits of \hat{X} and \hat{Z} placing the former at the end of the binary expansion, thereby embedding \hat{X} within \hat{Z} . This way, \hat{X} can be reconstructed from \hat{Z} , and adding noise gives a distribution that is absolutely continuous with respect to Lebesgue measure. By making the truncation point sufficiently far down the expansions, we can ensure the ϵ proximity required.

For a general rejection region, we first approximate it using a finite union of boxes. Much of the work in the proof then goes into controlling the approximation error. This is achieved by considering a large number of potential embeddings for which the supports of the resulting distributions have little overlap, and using a probabilistic argument.

3 The Generalised Covariance Measure

We have seen how conditional independence testing is not possible without restricting the null hypothesis. In this section we give a general construction for a conditional independence test based on regression procedures for regressing $\mathbf{Y}^{(n)}$ and $\mathbf{X}^{(n)}$ on $\mathbf{Z}^{(n)}$. In the case where

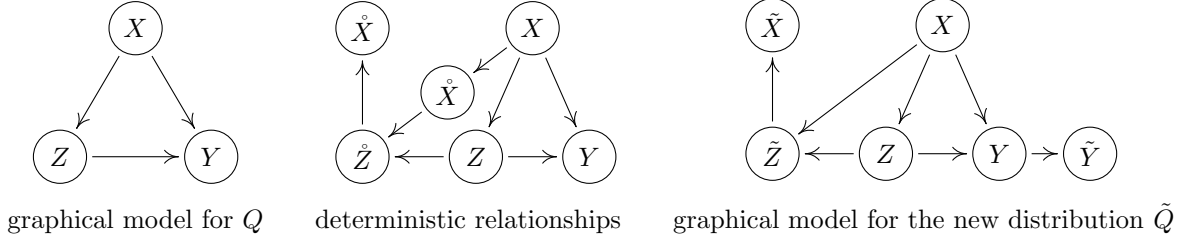


Figure 1: Illustration of the main idea of the proof of Theorem 2. Left: We start with a distribution $Q \in \mathcal{Q}_{0,M}$ over (X, Y, Z) . In general, the Q is Markov only to a fully connected graphical model. Middle: After discretising X to \tilde{X} , we are able to “hide” variable \tilde{X} in $\tilde{Z} = f(Z, \tilde{X})$ such that variable \tilde{Z} is close to Z in ℓ_∞ -norm and \tilde{X} can be reconstructed from \tilde{Z} . Thus, \tilde{X} , does not contain any “additional information” about Y when conditioning on \tilde{Z} . Right: We then consider noisy versions of the variables to guarantee that the new distribution P (over $\tilde{X}, \tilde{Y}, \tilde{Z}$) is absolutely continuous with respect to Lebesgue measure, and has $\tilde{X} \perp\!\!\!\perp \tilde{Y} \mid \tilde{Z}$. (The noise in \tilde{Z} is such that it still allows us to reconstruct \tilde{X} from \tilde{Z} .)

$d_X = d_Y = 1$, which we treat in the next section, the basic form of our test statistic is a normalised covariance between the residuals from these regressions. Because of this, we call our test statistic the *generalised covariance measure* (GCM). In Section 3.2 we show how to extend the approach to handle cases where more generally $d_X, d_Y \geq 1$.

3.1 Univariate X and Y

Given a distribution P for (X, Y, Z) , we can always decompose

$$X = f_P(Z) + \varepsilon_P, \quad Y = g_P(Z) + \xi_P,$$

where $f_P(z) = \mathbb{E}_P(X|Z = z)$ and $g_P(z) = \mathbb{E}_P(Y|Z = z)$. Similarly, for $i = 1, 2, \dots$ we define $\varepsilon_{P,i}$ and $\xi_{P,i}$ by $x_i - f_P(z_i)$ and $y_i - g_P(z_i)$ respectively. Also let $u_P(z) = \mathbb{E}_P(\varepsilon_P^2|Z = z)$ and $v_P(z) = \mathbb{E}_P(\xi_P^2|Z = z)$.

Let $\hat{f}^{(n)}$ and $\hat{g}^{(n)}$ be estimates of the conditional expectations f_P and g_P formed, for example, by regressing $\mathbf{X}^{(n)}$ and $\mathbf{Y}^{(n)}$ on $\mathbf{Z}^{(n)}$. For $i = 1, \dots, n$, we compute the product between residuals from the regressions:

$$R_i = \{x_i - \hat{f}(z_i)\}\{y_i - \hat{g}(z_i)\}. \quad (2)$$

Here, and in what follows, we have sometimes suppressed dependence on n and P for simplicity of presentation. We then define $T^{(n)}$ to be a normalised sum of the R_i ’s:

$$T^{(n)} = \frac{\sqrt{n} \cdot \frac{1}{n} \sum_{i=1}^n R_i}{\left(\frac{1}{n} \sum_{i=1}^n R_i^2 - \left(\frac{1}{n} \sum_{r=1}^n R_r \right)^2 \right)^{1/2}} =: \frac{\tau_N^{(n)}}{\tau_D^{(n)}}. \quad (3)$$

Our final test can be based on $|T^{(n)}|$ with large values suggesting rejection. Note that the introduction of notation for the numerator and denominator in the definition of $T^{(n)}$ are for later use in Theorem 8.

In the case where \hat{f} and \hat{g} are formed through linear regressions, the test is similar to one based on partial correlation, and would be identical were the denominator in (3) to be replaced by the the product of the empirical standard deviations of the vectors $(x_i - \hat{f}(z_i))_{i=1}^n$ and $(y_i - \hat{g}(z_i))_{i=1}^n$. This approach however would fail for Example 1 despite f and g being linear (in fact both equal to the zero function) as the product of the variances of the residuals would not

in general equal the variance of their product. Indeed, the reader may convince herself using `ppcor.test` from the R package `ppcor` [31], for example, that common tests for vanishing partial correlation do not yield the correct size in this case.

The following result gives conditions under which when the null hypothesis of conditional independence holds, we can expect the asymptotic distribution of $T^{(n)}$ to be a standard normal.

Theorem 6. *Define the following quantities:*

$$\begin{aligned} A_f &:= \frac{1}{n} \sum_{i=1}^n \{f_P(z_i) - \hat{f}(z_i)\}^2, & B_f &:= \frac{1}{n} \sum_{i=1}^n \{f_P(z_i) - \hat{f}(z_i)\}^2 v_P(z_i), \\ A_g &:= \frac{1}{n} \sum_{i=1}^n \{g_P(z_i) - \hat{g}(z_i)\}^2, & B_g &:= \frac{1}{n} \sum_{i=1}^n \{g_P(z_i) - \hat{g}(z_i)\}^2 u_P(z_i). \end{aligned}$$

We have the following results:

- (i) *If for $P \in \mathcal{P}_0$, $A_f A_g = o_P(n^{-1})$, $B_f = o_P(1)$, $B_g = o_P(1)$ and also $0 < \mathbb{E}_P(\varepsilon_P^2 \xi_P^2) < \infty$, then*

$$\sup_{t \in \mathbb{R}} |\mathbb{P}_P(T^{(n)} \leq t) - \Phi(t)| \rightarrow 0.$$

- (ii) *Let $\mathcal{P} \subset \mathcal{P}_0$ be a class of distributions such that $A_f A_g = o_P(n^{-1})$, $B_f = o_P(1)$, $B_g = o_P(1)$. If in addition $\inf_{P \in \mathcal{P}} \mathbb{E}(\varepsilon_P^2 \xi_P^2) \geq c_1$ and $\sup_{P \in \mathcal{P}} \mathbb{E}_P\{(\varepsilon_P \xi_P)^{2+\eta}\} \leq c_2$ for some $c_1, c_2 > 0$ and $\eta > 0$, then*

$$\sup_{P \in \mathcal{P}} \sup_{t \in \mathbb{R}} |\mathbb{P}_P(T^{(n)} \leq t) - \Phi(t)| \rightarrow 0.$$

Remark 7. *Applying the Cauchy–Schwarz inequality and Markov’s inequality, we see the requirement that $A_f A_g = o_P(n^{-1})$ is fulfilled if*

$$n \mathbb{E}_P \left(\frac{1}{n} \sum_{i=1}^n \{f_P(z_i) - \hat{f}(z_i)\}^2 \right) \mathbb{E}_P \left(\frac{1}{n} \sum_{i=1}^n \{g_P(z_i) - \hat{g}(z_i)\}^2 \right) \rightarrow 0. \quad (4)$$

Thus if in addition we have $\mathbb{E}_P B_f, \mathbb{E}_P B_g \rightarrow 0$, this is sufficient for all conditions required in (i) to hold.

If $\mathbb{E}_P B_f, \mathbb{E}_P B_g$ and the left-hand side of (4) converges to 0 uniformly over all $P \in \mathcal{P}$, then the conditions in (ii) will hold provided the moment condition on $\varepsilon_P \xi_P$ is also satisfied.

A proof is given in the supplementary material. We see that under conditions largely to do with the mean squared prediction error (MSPE) of \hat{f} and \hat{g} , $T^{(n)}$ can be shown to be asymptotically standard normal (i), and if the prediction error is uniformly small, the convergence to the Gaussian limit is correspondingly uniform (ii). A key point is that the requirement on the predictive properties of \hat{f} and \hat{g} is reasonably weak: for example, provided their MSPEs are $o(n^{-1/2})$, we have that the condition on $A_f A_g$ is satisfied. If in addition $\max_{i=1}^n |v_P(z_i)|$ and $\max_{i=1}^n |u_P(z_i)|$ are $O_P(\sqrt{n})$, then the conditions on B_f and B_g will be automatically satisfied. The latter conditions would hold if $\mathbb{E}_P u_P^2(Z) < \infty$ and $\mathbb{E}_P v_P^2(Z) < \infty$, for example.

Note that the rate of convergence requirement on A_f and A_g is a slower rate of convergence than required for estimating Lipschitz regression functions when $d_Z = 1$, for example. Indeed, we show more generally in Section 4 that f and g being in a reproducing kernel Hilbert space (RKHS) is enough for them to be estimable at the required rate.

In the setting where Z is high-dimensional and f and g are sparse and linear, standard theory for the Lasso [53, 10] shows that it may be used to obtain estimates \hat{f} and \hat{g} satisfying

the required properties under appropriate sparsity conditions. In fact, in this case our test statistic is closely related to that involved in the ANT procedure of [45] and the so-called RP test introduced in [51], which amount to a regularised partial correlation. A difference is that the denominator in (3) means the GCM test would not require $\varepsilon_P \perp\!\!\!\perp \xi_P$ unlike the ANT test and the RP test.

We now briefly sketch the reason for the relatively weak requirement on the MSPEs. In the following we suppress dependence on P for simplicity of presentation. We have

$$\begin{aligned} \frac{1}{\sqrt{n}} \sum_{i=1}^n R_i &= \frac{1}{\sqrt{n}} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i) + \varepsilon_i\} \{g(z_i) - \hat{g}(z_i) + \xi_i\} \\ &= (b + \nu_g + \nu_f) + \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i \xi_i, \end{aligned} \quad (5)$$

where

$$\begin{aligned} b &:= \frac{1}{\sqrt{n}} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i)\} \{g(z_i) - \hat{g}(z_i)\}, \\ \nu_g &:= \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i \{g(z_i) - \hat{g}(z_i)\} \quad \nu_f := \frac{1}{\sqrt{n}} \sum_{i=1}^n \xi_i \{f(z_i) - \hat{f}(z_i)\}. \end{aligned}$$

The summands in the final term in (5) are i.i.d. with zero mean provided $P \in \mathcal{P}_0$, so the central limit theorem dictates that these converge to a standard normal. We also see that the simple form of the GCM gives rise to the term b involving a product of bias-type terms from estimating f and g , so each term is only required to converge to 0 at a slow rate such that their product is of smaller order than the variance of the final term. The summands in ν_g are, under the null, mean zero conditional on $(\mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$. This term and similarly ν_f are therefore both relatively well-behaved, and give rise to the weak conditions on B_f and B_g .

3.1.1 Power of the GCM

We now present a result on the power of a version of the GCM. We may view our test statistic as a normalised version of the conditional covariance $\mathbb{E}_P(\varepsilon_P \xi_P) = \mathbb{E}_P \mathbf{cov}_P(X, Y|Z)$, where $\mathbf{cov}_P(X, Y|Z) = \mathbb{E}_P(XY|Z) - \mathbb{E}_P(X|Z)\mathbb{E}_P(Y|Z)$. This is always zero under the null, see Equation (1), and does not necessarily need to be non-zero under an alternative; we can only hope to have power against alternatives where this conditional covariance is non-zero.

Control of the term b in (5) under the alternative can proceed in exactly the same way as under the null. However control of the terms ν_f and ν_g typically requires additional conditions (for example Donsker-type conditions) on the estimators \hat{f} and \hat{g} as under the alternative both the errors ε_i and \hat{g} can depend on $\mathbf{Y}^{(n)}$. A notable exception is when f and g are sparse linear functions; in this setting alternative arguments can be used to show the GCM with Lasso regressions has optimal power when Z has a sparse inverse covariance [45, 51].

To state a general result avoiding additional conditions, here we will suppose that \hat{f} and \hat{g} have been constructed from an auxiliary training sample, independent of the data $(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$, see, for example, [46, 56]. A drawback however, compared to the original GCM, is that the corresponding prediction error terms A_f and A_g are here out-of-sample prediction errors. These are typically more sensitive to the distribution of Z and larger than the in-sample prediction errors featuring in Theorem 6. For this reason we consider the sample splitting approach to be more of a tool to facilitate theoretical analysis and would usually recommend using the original GCM in practice due to its typically better type I error control.

Theorem 8. Consider the setup of Theorem 6 but with the following differences: \hat{f} and \hat{g} have been constructed using auxiliary data independent of $(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$; the null hypothesis \mathcal{P}_0 is replaced by \mathcal{E}_0 the set of all distributions absolutely continuous with respect to Lebesgue measure; and conditions involving $\varepsilon_P \xi_P$ are replaced by those involving the centred version $\varepsilon_P \xi_P - \mathbb{E}_P(\varepsilon_P \xi_P)$. Define

$$\rho_P = \mathbb{E}_P \mathbf{cov}_P(X, Y|Z) \quad \text{and} \quad \sigma_P = \sqrt{\mathbf{var}_P(\varepsilon_P \xi_P)}.$$

Then under the conditions of (i) in Theorem 6 we have

$$\sup_{t \in \mathbb{R}} \left| \mathbb{P}_P \left(\frac{\tau_N^{(n)} - \sqrt{n} \rho_P}{\tau_D^{(n)}} \leq t \right) - \Phi(t) \right| \rightarrow 0, \quad \tau_D^{(n)} - \sigma_P = o_P(1),$$

with $\tau_N^{(n)}$ and $\tau_D^{(n)}$ defined as in (3).

Under the conditions of (ii) in Theorem 6 we have

$$\sup_{P \in \mathcal{P}} \sup_{t \in \mathbb{R}} \left| \mathbb{P}_P \left(\frac{\tau_N^{(n)} - \sqrt{n} \rho_P}{\tau_D^{(n)}} \leq t \right) - \Phi(t) \right| \rightarrow 0, \quad \tau_D^{(n)} - \sigma_P = o_P(1).$$

A proof is given in the supplementary material. We see that we achieve optimal \sqrt{n} rates for estimating ρ_P .

3.1.2 Relationship to semiparametric models

In viewing $\tau_N^{(n)}/\sqrt{n}$ as an estimator of the functional ρ_P , our GCM test connects to a vast literature in semiparametric statistics. In particular, the requirement of estimating nonparametric quantities (in our case $\sqrt{A_f}$ and $\sqrt{A_g}$) at a $o(n^{-1/4})$ rate is common for estimators of functionals based on estimating equations involving influence functions [7]. Our requirement on prediction error necessitates that at least one of f_P and g_P is Hölder β -smooth with $\beta/(2\beta + d_Z) \geq 1/4$. Estimators of the expected conditional covariance functional requiring minimal possible smoothness conditions may be derived using the theory of higher order influence functions [46, 47, 38, 48]; these estimators are however more complicated, and require some base nonparametric estimators used in their construction to satisfy conditions other than performing well in terms of prediction. Newey and Robins [40] study another approach to estimation of the functional based on a particular spline-based regression method. The work of Chernozhukov et al. [15] uses related ideas to ours here to obtain $1/\sqrt{n}$ convergent estimates and confidence intervals for parameters such as average treatment effects in causal inference settings. A distinguishing feature of our work here is that we only require in-sample prediction error bounds under the null of conditional independence, which is advantageous in our setting for the reasons mentioned in the previous section.

3.2 Multivariate X and Y

We now consider the more general setting where $d_X, d_Y \geq 1$. We let $T_{jk}^{(n)}$ be the univariate GCM based on data $(\mathbf{X}_j^{(n)}, \mathbf{Y}_k^{(n)}, \mathbf{Z}^{(n)})$ and regression methods \hat{f}_j and \hat{g}_k . (As described in Section 1.4, the subindex selects a column.) More generally, we will add subscripts j and k to certain terms defined in the previous subsection to indicate that the quantities are based on X_j and Y_k rather than X and Y . Thus, for example, $\varepsilon_{P,j}$ is the difference of X_j and its conditional expectation given Z .

We define our aggregated test statistic to be

$$S_n = \max_{j=1,\dots,d_X, k=1,\dots,d_Y} |T_{jk}^{(n)}|.$$

There are other choices for how to combine the test statistics in $\mathbf{T}^{(n)} := (T_{jk}^{(n)})_{j,k} \in \mathbb{R}^{d_X \cdot d_Y}$ into a single test statistic. Under similar conditions to those in Theorem 6, one can show that if d_X and d_Y are fixed, $\mathbf{T}^{(n)}$ will converge in distribution to a multivariate Gaussian limit with a covariance that can be estimated. The continuous mapping theorem can then be used to deduce the asymptotic limit distribution of the sum of squares of $T_{jk}^{(n)}$, for example. However, one advantage of the maximum is that the bias component of S_n will be bounded by the maximum of the bias terms in $T_{jk}^{(n)}$. A sum of squares-type statistic would have a larger bias component, and tests based on it may not maintain the level for moderate to large d_X or d_Y . Furthermore, S_n will tend to exhibit good power against alternatives where conditional independence is only violated for a few pairs (X_j, Y_k) , i.e., when the set of (j, k) such that $X_j \not\perp Y_k | Z$ is small.

In order to understand what values of S_n indicate rejection, we will compare S_n to

$$\hat{S}_n = \max_{j=1,\dots,d_X, k=1,\dots,d_Y} |\hat{T}_{jk}^{(n)}|$$

where $\hat{\mathbf{T}}^{(n)} \in \mathbb{R}^{d_X \cdot d_Y}$ is mean zero multivariate Gaussian with a covariance matrix $\hat{\Sigma} \in \mathbb{R}^{d_X \cdot d_Y \times d_X \cdot d_Y}$ determined from the data as follows. Let $\mathbf{R}_{jk} \in \mathbb{R}^n$ be the vector of products of residuals (2) involved in constructing the test statistic $T_{jk}^{(n)}$. We set $\hat{\Sigma}_{jk,lm}$ to be the sample correlation between $\mathbf{R}_{jk} \in \mathbb{R}^n$ and \mathbf{R}_{lm} :

$$\hat{\Sigma}_{jk,lm} = \frac{\mathbf{R}_{jk}^T \mathbf{R}_{lm} - \bar{\mathbf{R}}_{jk} \bar{\mathbf{R}}_{lm}}{(\|\mathbf{R}_{jk}\|_2^2/n - \bar{\mathbf{R}}_{jk}^2)^{1/2} (\|\mathbf{R}_{lm}\|_2^2/n - \bar{\mathbf{R}}_{lm}^2)^{1/2}}.$$

Here $\bar{\mathbf{R}}_{jk}$ is the sample mean of the components of \mathbf{R}_{jk} .

Let \hat{G} be the quantile function of \hat{S}_n . This is a random function that depends on the data $(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$ through $\hat{\Sigma}$. Note that given the \mathbf{R}_{jk} , we can approximate \hat{G} to any degree of accuracy via Monte Carlo.

The ground-breaking work of Chernozhukov et al. [14] gives conditions under which \hat{G} can well-approximate the quantile function of a version of S_n where all bias terms, that is terms corresponding to b , ν_g and ν_f are all equal to 0. We will require that those conditions are met by $\varepsilon_{P,j} \xi_{P,k}$ for all $j = 1, \dots, d_X$, $k = 1, \dots, d_Y$ and $P \in \mathcal{P}$. Below, we lay out these conditions, which take two possible forms.

$$(A1a) \quad \max_{r=1,2} \mathbb{E}_P(|\varepsilon_{P,j} \xi_{P,k}|^{2+r}/C_n^r) + \mathbb{E}_P(\exp(|\varepsilon_{P,j} \xi_{P,k}|/C_n)) \leq 4;$$

$$(A1b) \quad \max_{r=1,2} \mathbb{E}_P(|\varepsilon_{P,j} \xi_{P,k}|^{2+r}/C_n^{r/2}) + \mathbb{E}_P(\max_{j,k} |\varepsilon_{P,j} \xi_{P,k}|^4/C_n^2) \leq 4;$$

$$(A2) \quad C_n^4 (\log(d_X d_Y n))^7 / n \leq C n^{-c} \text{ for some constants } C, c > 0 \text{ independent of } P \in \mathcal{P}.$$

The result below shows that under the moment conditions above, provided the prediction error following the regressions goes to zero sufficiently fast, \hat{G} closely approximates the quantile function of S_n and therefore may be used to correctly calibrate our test.

Theorem 9. *Suppose for $\mathcal{P} \subset \mathcal{P}_0$, that one of (A1a) and (A2b) hold, and that (A2) holds. Suppose that*

$$\max_{j,k} A_{f,j} A_{g,k} = o_{\mathcal{P}}(n^{-1} \log(d_X d_Y)^{-1/2}), \quad (6)$$

$$\max_j B_{f,j} = o_{\mathcal{P}}(\log(d_X d_Y)^{-2}), \quad \text{and} \quad \max_k B_{g,k} = o_{\mathcal{P}}(\log(d_X d_Y)^{-2}). \quad (7)$$

Suppose further that there exist sequences $(\tau_{f,n})_{n \in \mathbb{N}}$, $(\tau_{g,n})_{n \in \mathbb{N}}$ such that

$$\max_{i,j} |\varepsilon_{P,ij}| = O_{\mathcal{P}}(\tau_{g,n}), \quad \max_k A_{g,k} = o_{\mathcal{P}}(\tau_{g,n}^{-2} \log(d_X d_Y)^{-3}) \quad (8)$$

$$\max_{i,k} |\xi_{P,ik}| = O_{\mathcal{P}}(\tau_{f,n}), \quad \max_j A_{f,j} = o_{\mathcal{P}}(\tau_{f,n}^{-2} \log(d_X d_Y)^{-3}). \quad (9)$$

Then

$$\sup_{P \in \mathcal{P}} \sup_{\alpha \in (0,1)} |\mathbb{P}_P\{S_n \leq \hat{G}(\alpha)\} - \alpha| \rightarrow 0$$

A proof is given in the supplementary material.

Remark 10. If the errors $\{\varepsilon_{P,j}\}_{j=1}^{d_X}$ and $\{\xi_{P,k}\}_{k=1}^{d_Y}$ are all sub-Gaussian with parameters bounded above by some constant M uniformly across $P \in \mathcal{P}$, we may easily see that both (A1a) and (A1b) are satisfied with C_n a constant; see Chernozhukov et al. [14] for further discussion.

If additionally we have $A_{f,j}, A_{g,k} = o_{\mathcal{P}}(n^{-1/2} \log(d_X d_Y n)^{-4})$, (6), (8) and (9) will all be satisfied.

Theorem 9 allows for d_X and d_Y to be large compared to n . However the use of this result is not limited to these cases. In the univariate case or more generally when d_X and d_Y are small, one can consider mappings $f_X : \mathbb{R}^{d_X+d_Z} \rightarrow \mathbb{R}^{\tilde{d}_X}$ and $f_Y : \mathbb{R}^{d_Y+d_Z} \rightarrow \mathbb{R}^{\tilde{d}_Y}$ where \tilde{d}_X and \tilde{d}_Y are potentially large. Provided these mappings are not determined from the data, we will have for $\tilde{X} := f_X(X, Z)$ and $\tilde{Y} := f_Y(Y, Z)$ that $\tilde{X} \perp\!\!\!\perp \tilde{Y} | Z$ if $X \perp\!\!\!\perp Y | Z$ (see Equation (1)). Thus we may apply the methodology above to the mapped data, potentially allowing the test to have power against a more diverse set of alternatives. In view of Theorem 8, successful mappings should have the equivalent of ρ_P large, but also $\mathbb{E}(\tilde{X} | Z = \cdot)$ and $\mathbb{E}(\tilde{Y} | Z = \cdot)$ should not be so complex that it is impossible to estimate them well. We leave further investigation of this topic to further work.

4 GCM Based on Kernel Ridge Regression

We now apply the results of the previous section to a GCM based on estimating the conditional expectations via kernel ridge regression. For simplicity, we consider only the univariate case where $d_X = d_Y = 1$. In the following, we make use of the notation introduced in Section 3.1.

Given $\mathcal{P} \subset \mathcal{P}_0$, suppose that the conditional expectations f_P, g_P satisfy $f_P, g_P \in \mathcal{H}$ for some RKHS $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ with reproducing kernel $k : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}$. Let $K \in \mathbb{R}^{n \times n}$ have ij th entry $K_{ij} = k(z_i, z_j)/n$ and denote the eigenvalues of K by $\hat{\mu}_1 \geq \hat{\mu}_2 \geq \dots \geq \hat{\mu}_n \geq 0$. We will assume that under each $P \in \mathcal{P}$, k admits an eigen-expansion of the form

$$k(z, z') = \sum_{j=1}^{\infty} \mu_{P,j} e_{P,j}(z) e_{P,j}(z') \quad (10)$$

with orthonormal eigenfunctions $\{e_{P,j}\}_{j=1}^{\infty}$, so $\mathbb{E}_P e_{P,j} e_{P,k} = \mathbb{1}_{\{j=k\}}$, and summable eigenvalues $\mu_{P,1} \geq \mu_{P,2} \geq \dots \geq 0$. Such an expansion is guaranteed under mild conditions by Mercer's theorem.

Consider forming estimates $\hat{f} = \hat{f}^{(n)}$ and $\hat{g} = \hat{g}^{(n)}$ through kernel ridge regressions of $\mathbf{X}^{(n)}$ and $\mathbf{Y}^{(n)}$ on $\mathbf{Z}^{(n)}$ in the following way. For $\lambda > 0$, let

$$\hat{f}_{\lambda} = \operatorname{argmin}_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \{x_i - h(z_i)\}^2 + \lambda \|h\|_{\mathcal{H}}^2 \right\}.$$

We will consider selecting a final tuning parameter $\hat{\lambda}$ in the following data-dependent way:

$$\hat{\lambda} = \operatorname{argmin}_{\lambda > 0} \left\{ \frac{1}{n} \sum_{i=1}^n \frac{\hat{\mu}_i^2}{(\hat{\mu}_i + \lambda)^2} + \lambda \right\}.$$

The term minimised on the RHS is an upper bound on the mean-squared prediction error omitting constant factors depending on σ^2 (defined below in Theorem 11) and $\|f_P\|_{\mathcal{H}}^2$ or $\|g_P\|_{\mathcal{H}}^2$. Because of the hidden dependence on these quantities, this is not necessarily a practically effective way of selecting λ : our use of it here is simply to facilitate theoretical analysis. Finally define $\hat{f} = \hat{f}_{\hat{\lambda}}$, and define \hat{g} analogously. We will write $T^{(n)}$ for the test statistic formed as in (3) with these choices of \hat{f} and \hat{g} .

Theorem 11. *Let \mathcal{P} be such that $u_P(z), v_P(z) \leq \sigma^2$ for all z and $P \in \mathcal{P}$.*

- (i) *For any $P \in \mathcal{P}$, $\sup_{t \in \mathbb{R}} |\mathbb{P}_P(T^{(n)} \leq t) - \Phi(t)| \rightarrow 0$.*
- (ii) *Suppose $\sup_{P \in \mathcal{P}} \mathbb{E}_P\{(\varepsilon_P \xi_P)^{2+\eta}\} \leq c$ for some $c \geq 0$ and $\eta > 0$. Suppose further that $\sup_{P \in \mathcal{P}} \max(\|f_P\|_{\mathcal{H}}, \|g_P\|_{\mathcal{H}}) < \infty$ and*

$$\lim_{\lambda \downarrow 0} \sup_{P \in \mathcal{P}} \sum_{j=1}^{\infty} \min(\mu_{P,j}, \lambda) = 0. \quad (11)$$

Then

$$\sup_{P \in \mathcal{P}} \sup_{t \in \mathbb{R}} |\mathbb{P}_P(T^{(n)} \leq t) - \Phi(t)| \rightarrow 0.$$

A proof is given in the supplementary material.

Remark 12. *An application of dominated convergence theorem shows that a sufficient condition for (11) to hold is that $\sum_{j=1}^{\infty} \sup_{P \in \mathcal{P}} \mu_{P,j} < \infty$.*

The proof proceeds by first showing that the ridge regression estimators \hat{f} and \hat{g} satisfy $A_f A_g = o_P(n^{-1})$ and then applies Theorem 3.1. The requirement that f_P and g_P lie in an RKHS satisfying (10) is a rather weak regularity condition on the conditional expectations. For example, taking the Sobolev kernel shows that it is enough that the conditional expectations are Lipschitz when $d_Z = 1$. However, the uniformity offered by (ii) above requires $\sup_{P \in \mathcal{P}} \max(\|f_P\|_{\mathcal{H}}, \|g_P\|_{\mathcal{H}}) < \infty$ and a large value of $\sup_{P \in \mathcal{P}} \max(\|f_P\|_{\mathcal{H}}, \|g_P\|_{\mathcal{H}})$ will require a large sample size in order for $T^{(n)}$ to have a distribution close to a standard normal. We investigate this, and evaluate the empirical performance of the GCM in the next section.

5 Experiments

Section 3 proposes the generalised covariance measure (GCM). Although we provide detailed computations for kernel ridge regression in Section 4, the technique can be combined with any regression method. In practice, the choice may depend on external knowledge of the specific application the user has in mind. In this section, we study the empirical performance of the GCM with boosted regression trees as the regression method. In particular, we use the R package `xgboost` [13, 12] with a ten-fold cross-validation scheme over the parameter `maxdepth`.

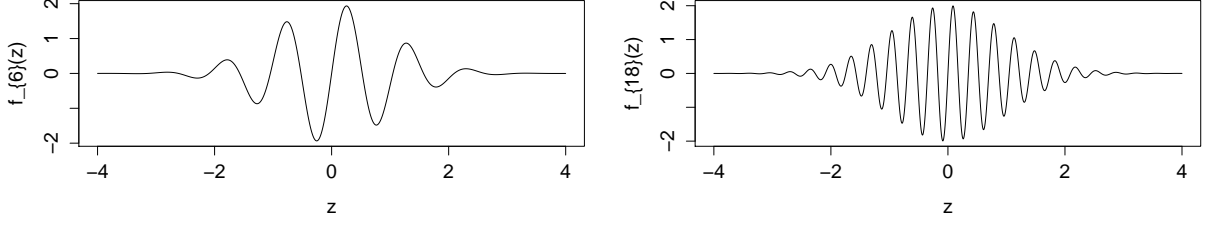


Figure 2: Graphs of the function f_a for $a = 6$ (left) and $a = 18$ (right). This function is used as the conditional mean that needs to be estimated from data. The RKHS norm increases exponentially with a , see (12).

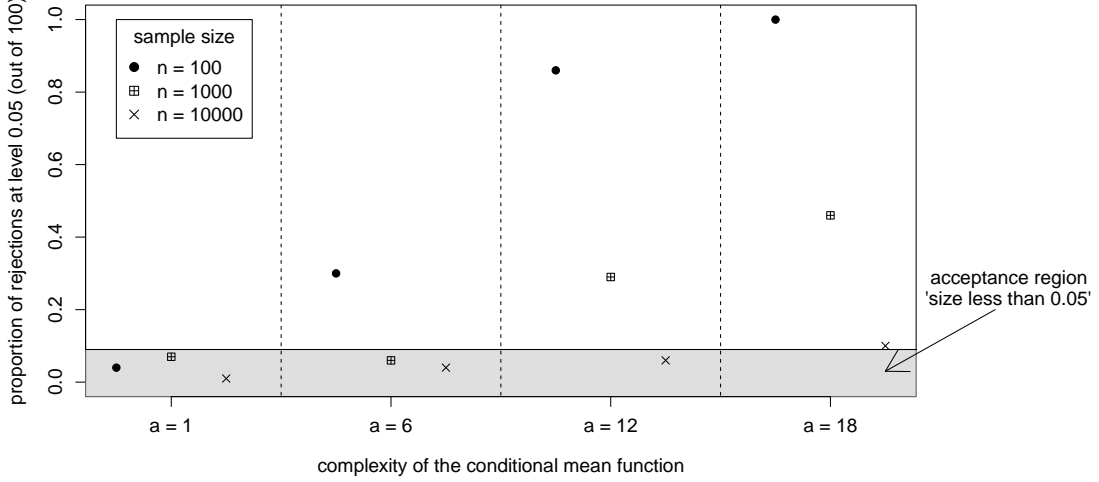


Figure 3: Illustration of the no-free-lunch theorem, see Section 5.1. No sample size is large enough to ensure the correct level for all distributions from the null: there is always a distribution from the null which yields a type I error that is larger than the prespecified significance level of 0.05. The shaded area indicates the area in which we accept the null hypothesis that the size of the test is less than 0.05.

5.1 No-free-lunch in Conditional Independence Testing

Theorem 2 states that if a conditional independence test has power against an alternative at a given sample size, then there is a distribution from the null that is rejected with probability larger than the significance level. Let us first fix an RKHS \mathcal{H} that corresponds to a Gaussian kernel with bandwidth $\sigma = 1$. We now compute for different sample sizes the rejection rates for data sets generated from the following model: $Z = N_Z$, $Y = f_a(Z) + N_Y$, and $X = f_a(Z) + N_X$, with $N_X, N_Y, N_Z \sim \mathcal{N}(0, 1)$, i.i.d., and $f_a(z) := \exp(-z^2/2) \sin(az)$. Figure 5.1 shows a plot of f_a for $a = 6$ and $a = 18$. Clearly, for any a , we have $X \perp\!\!\!\perp Y|Z$, but for large values of a the independence is harder to detect from data.

To illustrate the no-free-lunch theorem, we fix three different (large) sample sizes $n = 100$, $n = 1000$, and $n = 10000$. For any of such sample size n , we find an a , i.e., a distribution from the null, such that the probability of (falsely) rejecting $X \perp\!\!\!\perp Y|Z$ is larger than the prespecified level α . Figure 5.1 shows the results for the GCM test with boosted regression trees and the significance level $\alpha = 0.05$: for any sample size, we can choose a distribution from the null, for which the test rejects the null hypothesis of conditional independence. For $n = 100$, we can choose $a = 6$, for $n = 1000$, we choose $a = 12$, and for $n = 10000$, $a = 18$. This sequence of distributions violates one of the assumptions that we require for the GCM test to obtain

uniform asymptotic level guarantee: intuitively, the conditional expectations $z \mapsto \mathbb{E}[X|Z = z]$ and $z \mapsto \mathbb{E}[Y|Z = z]$ are too complex to be estimated reliably from the data. Formally, we can compute the RKHS norm of the functions f_a :

$$\|f_a\|_{\mathcal{H}}^2 = \int_{-\infty}^{\infty} F_a(\omega)^2 \exp(\sigma^2 \omega^2 / 2) d\omega = \sqrt{8\pi} \cdot (\exp(a^2) + \exp(-a^2)), \quad (12)$$

where

$$F_a(\omega) = \exp(-(\omega - a)^2 / 2) + \exp(-(\omega + a)^2 / 2)$$

is the Fourier transform of f_a . Equation (12) shows that a null hypothesis \mathcal{P} containing all of the above models for $a > 0$, violates one of the assumptions in Theorem 11: for this choice of RKHS and null hypothesis there is no M such that $\sup_{P \in \mathcal{P}} \max(\|f_P\|_{\mathcal{H}}, \|g_P\|_{\mathcal{H}}) < M$. (Not *all* sequences of functions with growing RKHS norm also yield a violation of level guarantees: some functions with large RKHS norm, e.g., modifications of constant functions, can be easily learned from data.) Other conditional independence tests fail on the examples in Figure 5.1, too, for a similar reason. However most of these other methods are less transparent in the underlying assumptions, since they do not come with uniform level guarantees.

5.2 On Level and Power

It is of course impossible to provide an exhaustive simulation-based level and power analysis. We therefore concentrate on a small choice of distributions from the null and the alternative. In the following, we compare the GCM with three other conditional independence tests: KCI [55] with its implementation from `CondIndTests` [27], and the residual prediction test [27, 51]. Finally, we also compare to a test that performs the same regression as GCM, but then tests for independence between the residuals, rather than vanishing correlation, using HSIC [26]. (This procedure is similar to the one that Fan et al. [21] propose to use in the case of additive noise models.) As we discuss in Example 1, we do not expect this test to hold level in general. We then generate distributions from the null:

- (a) $Z \sim \mathcal{N}(0, 1)$, $X = f_a(Z) + 0.3\mathcal{N}(0, 1)$, $Y = f_a(Z) + 0.3\mathcal{N}(0, 1)$, $a = 2$;
- (b) the same as (a) but with $a = 4$;
- (c) $Z_1, Z_2 \sim \mathcal{N}(0, 1)$ independent, $X = f_1(Z_1) - f_1(Z_2) + 0.3\mathcal{N}(0, 1)$, $Y = f_1(Z_1) + f_1(Z_2) + 0.3\mathcal{N}(0, 1)$;
- (d) $Z \sim \mathcal{N}(0, 1)$, $X_1 = f_1(Z) + 0.3\mathcal{N}(0, 1)$, $X_2 = f_1(Z) + X_1 + 0.3\mathcal{N}(0, 1)$, $Y_1 = f_1(Z) + 0.3\mathcal{N}(0, 1)$, $Y_2 = f_1(Z) + Y_1 + 0.3\mathcal{N}(0, 1)$; and
- (e) $Z \sim \mathcal{N}(0, 1)$, $Y = f_2(Z) \cdot \mathcal{N}(0, 1)$, $X = f_2(Z) \cdot \mathcal{N}(0, 1)$.

This is done for sample sizes 50, 100, 200, 300, and 400 and repeated 100 times. Figure 4 shows that the GCM indeed has promising behaviour in terms of type I error control. As expected, however, it requires the sample size to be big enough to obtain a reliable estimate for the conditional mean. The colours indicate rejection rates for 100 experiments. For rejection rates below 0.11 the hypothesis “the size of the test is less than 0.05” is not rejected at level 0.01 (pointwise).

We then investigate the power by altering the distributions above, such that the equation for Y has the additional term $+0.2X$ giving $X \not\perp Y | Z$ (for (d), we add the term $+0.2X_2$ to the equation of Y_2). Figure 5 shows empirical rejection rates.

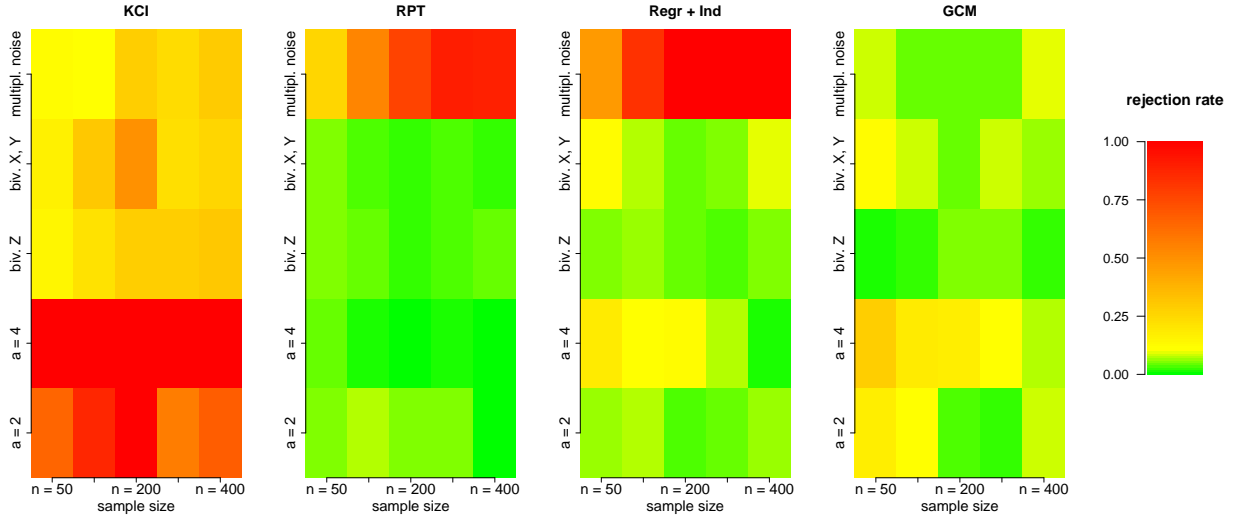


Figure 4: Level analysis: the GCM can hold the level if the sample size is large enough to reliably estimate the conditional mean. Testing for independence between residuals does not hold the level (third plot).

6 Discussion

A key result of this paper is that conditional independence testing is hard: non-trivial tests that maintain valid level over the entire class of distributions satisfying conditional independence and that are absolutely continuous with respect to Lebesgue measure cannot exist. In unconditional independence testing, control of type I error is straightforward and research efforts have focussed on power properties of tests. Our result indicates that in conditional independence testing, the basic requirement of type I error control deserves further attention. We argue that as domain knowledge is necessary in order to select a conditional independence test appropriate for a particular setting, there is a need to develop conditional independence tests whose suitability is reasonably straightforward to judge.

In this work we have introduced the GCM framework to address this need. The ability for the GCM to maintain the correct level relies almost exclusively on the predictive properties of the regression procedures upon which it is based. Selecting a good regression procedure, whilst mathematically an equally impossible problem, can at least be usefully informed by domain knowledge. We hope to see further applications of GCM-based tests in the future. On the theoretical side, it would be interesting to understand more precisely the tradeoff between the type I and type II errors in conditional independence testing. Often, work on testing fixes a null and then considers what sorts of classes of alternative distributions it is possible, or impossible to maintain power against. In the context of conditional independence testing, the problem set is even richer, in that one must also consider subclasses of null distributions, and can then study power properties associated with that null.

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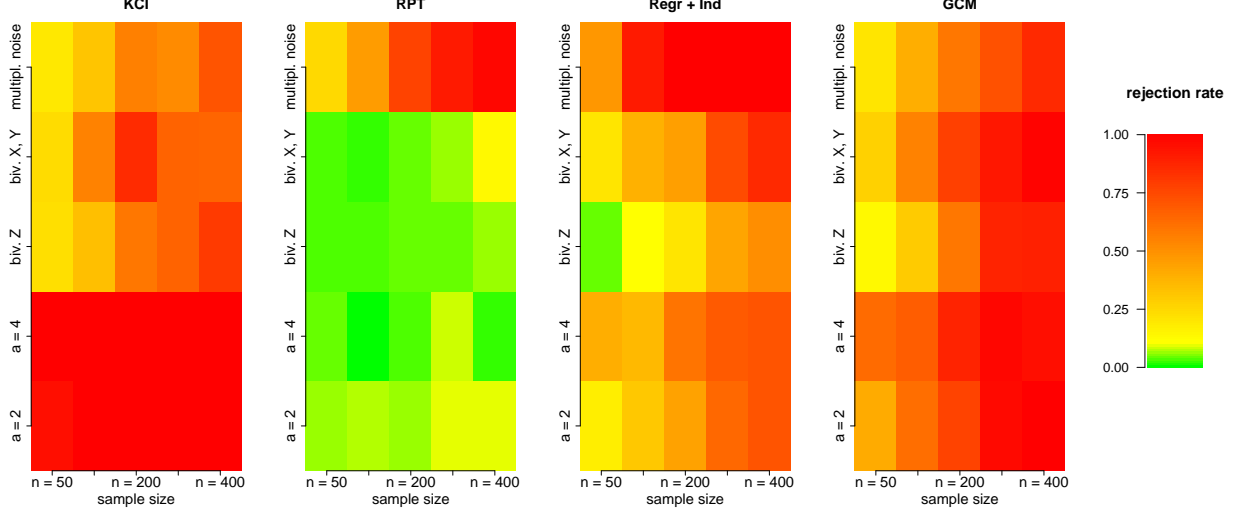


Figure 5: Power analysis: most of the methods are able to detect if the distribution does not satisfy conditional independence, in particular if the sample size increases.

his talks, e.g., at the Machine Learning Summer School in Tübingen in 2013. We thank Matey Neykov for kindly pointing out an error in the original version of this manuscript. We also thank Peter Bühlmann for helpful discussions regarding the aggregation of tests via taking the maximum test statistic.

A Proof of Theorem 2

The proof of Theorem 2 relies heavily on Lemma 13 in Section A.2, which shows that given any distribution Q where $(X, Y, Z) \sim Q$, one can construct $(\tilde{X}, \tilde{Y}, \tilde{Z})$ with $\tilde{X} \perp\!\!\!\perp \tilde{Y} | \tilde{Z}$ where $(\tilde{X}, \tilde{Y}, \tilde{Z})$ and (X, Y, Z) are arbitrarily close in ℓ_∞ -norm with arbitrarily high probability.

In the proofs of Theorem 2 and Lemma 13 below, we often suppress dependence n to simplify the presentation: thus for example, we write \mathbf{X} for $\mathbf{X}^{(n)}$. We use the following notation. We write $s = (d_X + d_Y + d_Z)$ and will denote by $V \in \mathbb{R}^s$ the triple (X, Y, Z) . Furthermore, $\mathbf{V} := (\mathbf{X}, \mathbf{Y}, \mathbf{Z})$. We denote by $p_{X,Y,Z}$ the density of (X, Y, Z) with respect to Lebesgue measure. We will use μ to denote Lebesgue measure on \mathbb{R}^{ns+1} and write \triangle for the symmetric difference operator.

A.1 Proof of Theorem 2

Suppose, for a contradiction, that there exists a Q with support strictly contained in an ℓ_∞ -ball of radius M under which $X \not\perp\!\!\!\perp Y | Z$ but $\mathbb{P}_Q(\psi_n(\mathbf{V}; U) = 1) = \beta > \alpha$. We will henceforth assume that $V \sim Q$ and $\mathbf{V} := (\mathbf{X}, \mathbf{Y}, \mathbf{Z})$ are i.i.d. copies of V . Thus we may omit the subscript Q applied to probabilities and expectations in the sequel. Denote the rejection region by

$$R = \{(\mathbf{x}, \mathbf{y}, \mathbf{z}; u) \in \mathbb{R}^{ns} \times [0, 1] : \psi_n(\mathbf{x}, \mathbf{y}, \mathbf{z}; u) = 1\}.$$

Our proof strategy is as follows. Using Lemma 13 we will create $\tilde{V} := (\tilde{X}, \tilde{Y}, \tilde{Z})$ such that $\tilde{X} \perp\!\!\!\perp \tilde{Y} | \tilde{Z}$ but \tilde{V} is suitably close to V such that a corresponding i.i.d. sample $\tilde{\mathbf{V}} := (\tilde{\mathbf{X}}, \tilde{\mathbf{Y}}, \tilde{\mathbf{Z}}) \in \mathbb{R}^{ns}$ satisfies $\mathbb{P}((\tilde{\mathbf{V}}, U) \in R) > \alpha$, contradicting that ψ_n has valid level α . How close \tilde{V} needs to be to V in order for this argument to work depends on the rejection region R . As an arbitrary

Borel subset of $\mathbb{R}^{ns} \times [0, 1]$, this can be arbitrarily complex; in order to get a handle on it we will construct an approximate version R^\sharp of R that is a finite union of boxes, see Lemma 15.

Let $\eta = (\beta - \alpha)/7 > 0$. Since $\{(x, y, z) : p_{X,Y,Z}(x, y, z) > m\} =: B_m \downarrow \emptyset$ as $m \uparrow \infty$, there exists M_1 such that $\mathbb{P}((X, Y, Z) \in B_{M_1}^c) > 1 - \eta/n$. Let Ω_1 be the event that $(x_i, y_i, z_i) \in B_{M_1}^c$ for all $i = 1, \dots, n$. (Here and below, an event refers to an element in the underlying σ -algebra. Recall that x_i, y_i , and z_i denote rows of \mathbf{X}, \mathbf{Y} , and \mathbf{Z} , respectively, i.e., they are random vectors.) Then by a union bound we have $\mathbb{P}(\Omega_1) \geq 1 - \eta$.

Let M_2 be such that $\mathbb{P}(\|\mathbf{V}\|_\infty > M_2) < \eta$ and let Ω_2 be the event that $\|\mathbf{V}\|_\infty \leq M_2$. Further define

$$\check{R} = \{(\mathbf{x}, \mathbf{y}, \mathbf{z}, u) \in R : \|(\mathbf{x}, \mathbf{y}, \mathbf{z})\|_\infty \leq M_2\}.$$

Note that

$$\mathbb{P}((\mathbf{V}, U) \in \check{R}) \geq \beta - \mathbb{P}((\mathbf{V}, U) \in R \setminus \check{R}) > \beta - \eta. \quad (13)$$

Let $L = L(\eta)$ be as defined in Lemma 13 (taking $\delta = \eta$). From Lemma 15 applied to \check{R} , we know there exists a finite union R^\sharp of hypercubes each of the form

$$\prod_{k=1, \dots, s+1} (a_k, b_k]$$

such that $\mu(R^\sharp \triangle \check{R}) < \eta / \max(L, M_1^n)$. By definition of Ω_1 we thus have that

$$\mathbb{P}(\{(\mathbf{V}, U) \in \check{R} \setminus R^\sharp\} \cap \Omega_1) < \eta. \quad (14)$$

Now for $r \geq 0$ and $\mathbf{v} \in \mathbb{R}^{ns+1}$ let $B_r(\mathbf{v}) \subseteq \mathbb{R}^{ns+1}$ denote the ℓ_∞ ball with radius $r > 0$ and center \mathbf{v} . Define

$$R^r = \{\mathbf{v} \in R : B_r(\mathbf{v}) \subseteq R^\sharp\}.$$

Then as $R^r \uparrow R^\sharp$ as $r \downarrow 0$, there exists $r_0 > 0$ such that $\mu(R^\sharp \setminus R^{r_0}) < \eta / M_1^n$.

For $\epsilon = r_0$ and $B = R^\sharp \setminus \check{R}$ the statement of Lemma 13 provides us with $\tilde{\mathbf{V}} := (\tilde{\mathbf{X}}, \tilde{\mathbf{Y}}, \tilde{\mathbf{Z}})$ which satisfies $\mathbb{P}((\tilde{\mathbf{V}}, U) \in R^\sharp \setminus \check{R}) < \eta$ and with which we argue as follows. Let Ω_3 be the event that $\|\mathbf{V} - \tilde{\mathbf{V}}\|_\infty < r_0$, so $\mathbb{P}(\Omega_3) \geq 1 - \eta$.

$$\begin{aligned} \mathbb{P}((\tilde{\mathbf{V}}, U) \in R) &\geq \mathbb{P}((\tilde{\mathbf{V}}, U) \in \check{R}) \geq \mathbb{P}((\tilde{\mathbf{V}}, U) \in R^\sharp) - \mathbb{P}((\tilde{\mathbf{V}}, U) \in R^\sharp \setminus \check{R}) \\ &> \mathbb{P}(\{(\tilde{\mathbf{V}}, U) \in R^\sharp\} \cap \Omega_3) - \eta > \mathbb{P}((\mathbf{V}, U) \in R^{r_0}) - 2\eta \\ &\geq \mathbb{P}((\mathbf{V}, U) \in R^\sharp) - \mathbb{P}(\{(\mathbf{V}, U) \in R^\sharp \setminus R^{r_0}\} \cap \Omega_1) - \mathbb{P}(\Omega_1^c) - 2\eta \\ &> \mathbb{P}((\mathbf{V}, U) \in R^\sharp) - 4\eta. \end{aligned}$$

Now

$$\begin{aligned} \mathbb{P}((\mathbf{V}, U) \in R^\sharp) &\geq \mathbb{P}((\mathbf{V}, U) \in \check{R}) - \mathbb{P}(\{(\mathbf{V}, U) \in \check{R} \setminus R^\sharp\} \cap \Omega_1) - \mathbb{P}(\Omega_1^c) \\ &> \mathbb{P}((\mathbf{V}, U) \in \check{R}) - 2\eta > \beta - 3\eta \end{aligned}$$

using (14) and (13). Putting things together, we have $\mathbb{P}((\tilde{\mathbf{V}}, U) \in R) > \beta - 7\eta > \alpha$, completing the proof.

A.2 Auxilliary Lemmas

Lemma 13. *Let (X, Y, Z) have a $(d_X + d_Y + d_Z)$ -dimensional distribution in $\mathcal{Q}_{0,M}$ for some $M \in (0, \infty]$. Let $(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)})$ be a sample of n i.i.d. copies of (X, Y, Z) . Given $\delta > 0$, there exists $L = L(\delta)$ such that for all $\epsilon > 0$ and all Borel subsets $B \subseteq \mathbb{R}^{n \cdot (d_X + d_Y + d_Z)} \times [0, 1]$, it is possible to construct n i.i.d. random vectors $(\tilde{\mathbf{X}}^{(n)}, \tilde{\mathbf{Y}}^{(n)}, \tilde{\mathbf{Z}}^{(n)})$ with distribution $P \in \mathcal{P}_{0,M}$ where the following properties hold:*

(i) $\mathbb{P}(\|(\mathbf{X}^{(n)}, \mathbf{Y}^{(n)}, \mathbf{Z}^{(n)}) - (\tilde{\mathbf{X}}^{(n)}, \tilde{\mathbf{Y}}^{(n)}, \tilde{\mathbf{Z}}^{(n)})\|_\infty < \epsilon) > 1 - \delta;$

(ii) If $U \sim U[0, 1]$ independently of $(\tilde{\mathbf{X}}^{(n)}, \tilde{\mathbf{Y}}^{(n)}, \tilde{\mathbf{Z}}^{(n)})$ then

$$\mathbb{P}((\tilde{\mathbf{X}}^{(n)}, \tilde{\mathbf{Y}}^{(n)}, \tilde{\mathbf{Z}}^{(n)}, U) \in B) \leq L\mu(B).$$

Proof. We will first describe the construction of $\tilde{V} := (\tilde{X}, \tilde{Y}, \tilde{Z})$ from $V := (X, Y, Z)$. The corresponding n -sample $\tilde{\mathbf{V}} := (\tilde{\mathbf{X}}^{(n)}, \tilde{\mathbf{Y}}^{(n)}, \tilde{\mathbf{Z}}^{(n)})$ will have observation vectors formed in the same way from the corresponding observation vectors in \mathbf{V} .

We begin by creating a bounded and discretised version of V , for which we can control an upper bound on the probability mass function. Define $s := d_X + d_Y + d_Z$. Since $\{(x, y, z) \in \mathbb{R}^s : p_{X,Y,Z}(x, y, z) > m\} =: B_m \downarrow \emptyset$ as $m \uparrow \infty$, there exists M_1 such that the event $\Lambda_1 = \{(X, Y, Z) \in B_{M_1}^c\}$ has $\mathbb{P}(\Lambda_1) \geq 1 - \delta/(2n)$. Next, let $M_2 < M$ be such that $\mathbb{P}(\|V\|_\infty > M_2) < \delta/(2n)$, and let Λ_2 be the event that $\|V\|_\infty \leq M_2$. For later use, we define the events

$$\Omega_1 = \{(x_i, y_i, z_i) \in B_{M_1}^c \text{ for all } i = 1, \dots, n\} \quad \text{and} \quad \Omega_2 = \{\|\mathbf{V}\|_\infty \leq M_2\}.$$

Note that union bounds give $\mathbb{P}((\Omega_1 \cap \Omega_2)^c) < \delta$.

Let $E^{(1)}$ be uniformly distributed on $[-M_2, M_2]^s$. Let $r \in \mathbb{N}$ be such that $2^{-r} < \min(\epsilon/(3n), (M - M_2)/3)$ and define

$$\tilde{V} := (\tilde{X}, \tilde{Y}, \tilde{Z}) := 2^{-r} \left\lfloor 2^r (V \mathbb{1}_{\Lambda_1 \cap \Lambda_2} + E^{(1)} \mathbb{1}_{(\Lambda_1 \cap \Lambda_2)^c}) \right\rfloor.$$

Here, the floor function is applied componentwise. Note that \tilde{V} takes values in a grid $(2^{-r}\mathbb{Z})^s$ and satisfies

$$\|(\tilde{V} - V) \mathbb{1}_{\Lambda_1 \cap \Lambda_2}\|_\infty \leq 2^{-r} < \epsilon/(3n). \quad (15)$$

The choice of r ensures that $\tilde{V} \in (-M', M')^s$ where $M' = M - 2(M - M_2)/3$. Furthermore, the inclusion of the $\mathbb{1}_{\Lambda_1 \cap \Lambda_2}$ term and $E^{(1)}$ ensures that the probability it takes any given value is bounded above by $M_3 2^{-sr}$ where $M_3 := M_1 + M_2^{-s}$. Note that M_3 does not depend on ϵ .

We can now apply Lemma 14 with $W = (\tilde{Y}, \tilde{Z})$ and $N = \tilde{X}$. This gives us $K!$ random vectors $\tilde{V}^{(1)}, \dots, \tilde{V}^{(K!)}$ where $K > 2^r$; for each $k = 1, \dots, K!$, $\tilde{V}^{(k)} = (\tilde{X}^{(k)}, \tilde{Y}^{(k)}, \tilde{Z}^{(k)})$ satisfies

- (a) $\mathbb{P}(|\tilde{V}_s^{(k)} - \tilde{V}_s| \leq 2^{-r}) = 1$ and $\tilde{V}_j^{(k)} = \tilde{V}_j$ for $j \leq s - 1$;
- (b) $\tilde{X}^{(k)}$ may be recovered from $\tilde{Z}^{(k)}$ via $\tilde{X}^{(k)} = \tilde{g}_k(\tilde{Z}^{(k)})$ for some function \tilde{g}_k ;
- (c) $\tilde{V}_s^{(k)}$ takes values in $K^{-2} 2^{-r} \mathbb{Z}$;
- (d) $\tilde{V}_s^{(k)}$ lies in $K^{-2} 2^{-r} \mathbb{Z}$ and the probability that $\tilde{V}^{(k)}$ takes any given value is bounded above by $2^{-sr} K^{-1} M_3$;

and, additionally,

- (d) the supports $\tilde{S}_1, \dots, \tilde{S}_{K!}$ of $\tilde{V}^{(1)}, \dots, \tilde{V}^{(K!)}$ obey the following structure: there exists a collection of K^2 disjoint sets $\{\tilde{G}_{jk}\}_{j,k=1}^K$ and an enumeration $\pi_1, \dots, \pi_{K!}$ of the permutations of $\{1, \dots, K\}$ such that $\tilde{S}_j = \cup_{k=1}^K \tilde{G}_{k\pi_j(k)}$ and $\mathbb{P}(\tilde{V}^{(j)} \in \tilde{G}_{k\pi_j(k)}) = K^{-1}$ for $j = 1, \dots, K!$.

We now create a noisy version of the $\tilde{V}^{(k)}$ that obeys similar properties to the above, but is absolutely continuous with respect to Lebesgue measure. To this end, we introduce $E^{(2)} = (E_X, E_Y, E_Z) \in (0, 1)^s$ with independent $U(0, 1)$ components. Then let $\tilde{V}^{(k)} \in \mathbb{R}^s$ be defined by

$$\tilde{V}_j^{(k)} = \begin{cases} K^{-2} 2^{-r} E_s^{(2)} + \tilde{V}_s^{(k)} & \text{for } j = s \\ 2^{-r} E_j^{(2)} + \tilde{V}_j^{(k)} & \text{otherwise.} \end{cases}$$

This obeys

- (a') $\mathbb{P}(\|\tilde{V}^{(k)} - \hat{V}^{(k)}\|_\infty \leq 2^{-r}) = 1$;
- (b') $\tilde{X}^{(k)}$ may be recovered from $\tilde{Z}^{(k)}$ via $\tilde{X}^{(k)} = g_k(\tilde{Z}^{(k)})$ for some function g_k ;
- (c') the density of $\tilde{V}^{(k)}$ with respect to Lebesgue measure is bounded above by KM_3 ;
- (d') the supports $S_1, \dots, S_{K!}$ of the $\{\tilde{V}^{(k)}\}_{k=1}^{K!}$ obey property (d) with the disjoint sets \tilde{G}_{jk} above replaced by another collection $\{G_{jk}\}_{j,k=1}^{K^2}$ of K^2 disjoint sets whose union is $(-M, M)^s$.

From (a'), by the triangle inequality we have that

$$\mathbb{P}(\|(\tilde{V}^{(k)} - V)\mathbb{1}_{\{\Lambda_1 \cap \Lambda_2\}}\|_\infty \leq \epsilon/n) = 1 \quad (16)$$

and $\tilde{V}^{(k)} \in (-M, M)^s$.

Note that (b') holds as the additional uniform noise can be removed by truncating its binary expansion appropriately. A consequence of this property is that decomposing $(\tilde{X}^{(k)}, \tilde{Y}^{(k)}, \tilde{Z}^{(k)}) = \tilde{V}^{(k)}$, we have $\tilde{X}^{(k)} \perp\!\!\!\perp \tilde{Y}^{(k)} | \tilde{Z}^{(k)}$. To see this we argue as follows. Let us write p_A and $p_{A|B}$ for the densities of A and A given B respectively when A and B are random vectors. Suppressing dependence on k temporarily, we have that for any \tilde{z} with $p_{\tilde{Z}}(\tilde{z}) > 0$,

$$\begin{aligned} p_{\tilde{X}, \tilde{Y}, \tilde{Z}}(\tilde{x}, \tilde{y} | \tilde{z}) &= p_{E_X, \tilde{Y} | \tilde{Z}}(\tilde{x} - g(\tilde{z}), \tilde{y} | \tilde{z}) = p_{E_X}(\tilde{x} - g(\tilde{z})) p_{\tilde{Y} | \tilde{Z}}(\tilde{y} | \tilde{z}) \\ &= p_{\tilde{X} | \tilde{Z}}(\tilde{x} | \tilde{z}) p_{\tilde{Y} | \tilde{Z}}(\tilde{y} | \tilde{z}). \end{aligned}$$

Thus, using [17], $\tilde{X} \perp\!\!\!\perp \tilde{Y} | \tilde{Z}$.

Let $\{\tilde{\mathbf{V}}^{(k)}\}_{k=1}^{K!}$ be the corresponding n -sample versions of $\{\tilde{V}^{(k)}\}_{k=1}^{K!}$. Then for any k , (16) and the triangle inequality gives $\mathbb{P}(\|(\tilde{\mathbf{V}}^{(k)} - \mathbf{V})\mathbb{1}_{\Omega_1 \cap \Omega_2}\|_\infty \leq \epsilon) = 1$. Thus $\mathbb{P}(\|\tilde{\mathbf{V}}^{(k)} - \mathbf{V}\|_\infty \leq \epsilon) > 1 - \delta$. We see that any $\tilde{\mathbf{V}}^{(k)}$ satisfies all requirements of the result except potentially (ii). In order to pick a k for which (ii) is satisfied, we use the so-called probabilistic method. First note we may assume $0 < \mu(B) < \infty$ or otherwise any k will do. Define $T_k := S_k^n \times [0, 1]$ to be the support set of $(\tilde{\mathbf{V}}^{(k)}, U)$ where $U \sim U[0, 1]$ independently of $\{\tilde{\mathbf{V}}^{(k)}\}_{k=1}^{K!}$.

For $j \in \{1, \dots, K\}$ let $G_j := \cup_{k=1}^K G_{jk}$. Let \mathcal{J} be the set of n -tuples (j_1, \dots, j_n) of distinct elements of $\{1, \dots, K\}$. Now define

$$C = \bigcup_{(j_1, \dots, j_n) \in \mathcal{J}} \prod_{l=1}^n G_{j_l}.$$

Let $D = C \times [0, 1]$. For all $(j_1, \dots, j_n) \in \mathcal{J}$ and any $(k_l)_{l=1}^n \in \{1, \dots, K\}^n$, $\prod_{l=1}^n G_{j_l k_l}$ is contained in some S_m^n precisely when for all l , we have $k_l = \pi_m(j_l)$. Thus there are $(K - n)!$ different products of support sets S_m^n that contain any given $\prod_{l=1}^n G_{j_l k_l} \subset C$. We therefore have that for any $\prod_{l=1}^n G_{j_l k_l} \subset C$ that

$$\sum_{k=1}^{K!} \mu \left\{ \left(\prod_{l=1}^n G_{j_l k_l} \right) \times [0, 1] \cap B \cap T_k \right\} \leq (K - n)! \mu \left\{ \left(\prod_{l=1}^n G_{j_l k_l} \right) \times [0, 1] \cap B \right\}.$$

Summing over all $\prod_{l=1}^n G_{j_l k_l} \subset C$ we obtain

$$\sum_{k=1}^{K!} \mu(B \cap D \cap T_k) \leq (K - n)! \mu(B \cap D) \leq (K - n)! \mu(B).$$

This gives that there exists at least one $k = k^*$ with

$$\mu(B \cap D \cap T_{k^*}) \leq \frac{(K - n)!}{K!} \mu(B).$$

Next, observe that the number of cells $\prod_{l=1}^n G_{j_l}$ where at least two of j_1, \dots, j_n are the same is $K^n - K(K-1)\dots(K-n+1)$. As $\mathbb{P}(\tilde{V}^{(k)} \in G_j) = K^{-1}$, we have for any k that

$$\mathbb{P}((\tilde{V}^{(k)}, U) \notin D) = K^{-n} \{K^n - K(K-1)\dots(K-n+1)\} = O(K^{-1}).$$

Putting things together we have that there must exist a k^* with

$$\begin{aligned} \mathbb{P}((\tilde{V}^{(k^*)}, U) \in B) &\leq \mathbb{P}((\tilde{V}^{(k^*)}, U) \in B \cap D) + \mathbb{P}((\tilde{V}^{(k^*)}, U) \notin D) \\ &\leq K^n M_3^n \frac{(K-n)!}{K!} \mu(B) + O(K^{-1}) \leq 2M_3^n \mu(B) \end{aligned}$$

for K sufficiently large, which can be arranged by taking r sufficiently large. \square

Lemma 14. *Let $W \in \mathbb{R}^m$, $N \in \mathbb{R}^d$ be random vectors. Suppose that N is bounded and there is some $r \in \mathbb{N}$ such that both W and N have components taking values in the grid $(2^{-r}\mathbb{Z})$. Suppose further that the probability that (N, W) takes any particular value is bounded by $2^{-(m+d)r}M$ for some $M > 0$. Then there exists a $K \in \mathbb{N}$ with $K > 2^r$ and a set of $K!$ functions $\{f_1, \dots, f_{K!}\}$ where*

$$(W_m, N) \mapsto f_k(W_m, N) =: \mathring{W}_m^{(k)} \in \mathbb{R}$$

such that for each $k = 1, \dots, K!$,

- (i) $\mathbb{P}(|W_m - \mathring{W}_m^{(k)}| \leq 2^{-r}) = 1$;
- (ii) there is some function $g_k : \mathbb{R} \rightarrow \mathbb{R}^d$ such that $N = g_k(\mathring{W}_m^{(k)})$;
- (iii) $\mathring{W}_m^{(k)}$ has components taking values in a grid $K^{-2}2^{-r}\mathbb{Z}$.

Moreover, defining $\mathring{W}^{(k)} = (W_1, \dots, W_{m-1}, \mathring{W}_m^{(k)})$,

- (iv) the probability that $(N, \mathring{W}^{(k)})$ takes any value is bounded above by $K^{-1}2^{-(m+d)r}M$;
- (v) the supports $S_1, \dots, S_{K!}$ of $(N, \mathring{W}^{(1)}), \dots, (N, \mathring{W}^{(K!)})$ obey the following structure: there exists K^2 disjoint sets $\{G_{jk}\}_{j,k=1}^K$ and an enumeration $\pi_1, \dots, \pi_{K!}$ of the permutations of $\{1, \dots, K\}$ such that for all j , $S_j = \cup_{k=1}^K G_{k\pi_j(k)}$, and for all j and k , $\mathbb{P}((N, \mathring{W}^{(j)}) \in G_{k\pi_j(k)}) = K^{-1}$.

Proof. As N is bounded, by replacing $g_k(\cdot)$ by $g_k(\cdot) + v$ where $v \in \mathbb{R}^d$ is appropriately chosen with components in $2^{-r}\mathbb{Z}$, we may assume that N has non-negative components. Let $t \in \mathbb{N}$ be such that $2^t > 2^r \max(1, \|N\|_\infty)$. We shall prove the result with $K = 2^{dt}$.

Define the random variable \mathring{N} by

$$\mathring{N} = 2^r \sum_{j=0}^{d-1} 2^{tj} N_{j+1}.$$

This is a concatenation of the binary expansions of $2^r N_j \in \{0, 1, 2, \dots, 2^t - 1\}$ for $j = 1, \dots, d$. Observe that $\mathring{N} \in \{0, 1, \dots, K-1\}$ and that N_j may be recovered from \mathring{N} by examining its binary expansion. Indeed, $2^r N_j$ is the residue modulo 2^t of $\lfloor \mathring{N} / 2^{t(j-1)} \rfloor$.

For $j = \{0, 1, \dots, K-1\}$, let \tilde{N}_j be the residue of $\mathring{N} + j$ modulo K , so $\tilde{N}_j \in \{0, 1, \dots, K-1\}$. Also, for $k = \{0, 1, \dots, K-1\}$ let $\tilde{N}_{j,k} = \tilde{N}_j + Kk$. Let the random variable E be uniformly distributed on $\{0, 1, \dots, K-1\}$ independently of all other quantities. Now let $\pi_1, \dots, \pi_{K!}$ be an enumeration of the permutations of $\{0, \dots, K-1\}$. Finally, let $\mathring{N}_l = \tilde{N}_{\pi_l(E), E}$ for $l = 1, \dots, K!$.

The reason for this particular construction is that we can recover E from \mathring{N}_k (and k) via $E = \lfloor \mathring{N}_k / K \rfloor$, and thereby determine $\pi_k(E)$, which then reveals \mathring{N} and each of the individual N_j . In summary, this gives us $K!$ different embeddings of the vector N into a single random variable.

We may now define f_k by

$$f_k(W_m, N) = W_m + 2^{-r} K^{-2} \mathring{N}_k.$$

It is easy to see that (i) and (iii) are satisfied. Our construction allows N and E to be recovered from $f_k(W_m, N)$, and so also W_m may be found. Thus in particular (ii) is satisfied. Let us write g_k, h_k and l_k for the functions that when applied to $f_k(W_m, N)$, yield N, E and W_m respectively. Let us introduce the notation that for a vector $v \in \mathbb{R}^s$, $v_{-j} \in \mathbb{R}^{s-1}$ for $j = 1, \dots, s$ is the subvector of v where the j th component is omitted. Then we have

$$\begin{aligned} \mathbb{P}(N = n, \mathring{W}^{(k)} = w) &= \mathbb{P}(W_{-m} = w_{-m}, W_m = l_k(w_m), N = n, E = h_k(w_m)) \mathbb{1}_{\{g_k(w_m)=n\}} \\ &= K^{-1} \mathbb{P}(W_{-m} = w_{-m}, W_m = l_k(w_m), N = n) \mathbb{1}_{\{g_k(w_m)=n\}} \\ &\leq K^{-1} 2^{-(m+d)r} M, \end{aligned}$$

using the independence of E in the second line above. This gives (iv).

Note that the supports of the $(N, \tilde{N}_{j,k})$ are all disjoint as (j, k) can be recovered from $(N, \tilde{N}_{j,k})$. For $j, k = 0, 1, \dots, K-1$ let G_{jk} be the support set of

$$(N, \tilde{W}_{j,k}) := (N, W_1, \dots, W_{m-1}, W_m + 2^{-r} K^{-2} \tilde{N}_{j,k}).$$

From the above, we see that the $\{G_{jk}\}_{j,k=0}^{K-1}$ are all disjoint. Property (v) follows from noting that $\mathring{W}^{(l)} = \tilde{W}_{\pi_l(E), E}$. \square

The following well-known result appears for example in Weaver [54, Theorem 2.19].

Lemma 15. *Given any bounded Borel subset B of \mathbb{R}^d and any $\epsilon > 0$, there exists a finite union of boxes of the form*

$$B^\# = \bigcup_{i=1}^N \prod_{k=1}^d (a_{i,k}, b_{i,k}]$$

such that $\mu(B \triangle B^\#) \leq \epsilon$, where μ denotes Lebesgue measure and \triangle denotes the symmetric difference operator.

B KL-Separation of Null and Alternative

For distributions $P_1, P_2 \in \mathcal{E}_0$, let $\text{KL}(P_1 || P_2)$ denote the KL divergence from P_2 to P_1 , which we define to be $+\infty$ when P_1 is not absolutely continuous with respect to P_2 . The following result, which is proved in the supplementary material, shows that it is possible to choose $Q \in \mathcal{Q}_0$ that is arbitrarily far away from \mathcal{P}_0 (by picking $\sigma^2 > 0$ to be sufficiently small).

Proposition 16. *Consider the distribution Q over the triple $(X, Y, Z) \in \mathbb{R}^3$ defined in the following way: $Y = X + N$ with $X \sim \mathcal{N}(0, 1)$, $N \sim \mathcal{N}(0, \sigma^2)$ and $X \perp\!\!\!\perp N$. The variable $Z \sim \mathcal{N}(0, 1)$ is independent of (X, Y) . Thus $X \not\perp\!\!\!\perp Y | Z$, i.e., $Q \in \mathcal{Q}_0$, and we have*

$$\inf_{P \in \mathcal{P}_0} \text{KL}(Q || P) = \frac{1}{2} \log \left(\frac{1 + \sigma^2}{\sigma^2} \right) = \inf_{P \in \mathcal{P}_0} \text{KL}(P || Q).$$

Supplementary Material

This supplementary material contains the proofs of results omitted in the appendices A and B in the main paper.

C Proof of Additional Results in Sections 2 and B

C.1 Results on the Separation Between the Null and Alternative Hypotheses

In this section we provide proofs of Propositions 5 and 16.

C.1.1 Proof of Proposition 5

The proof of Proposition 5 makes frequent use of the following lemma.

Lemma 17. *Let probability measures P and Q be defined on $[-M, M]$. Then*

$$|\mathbb{E}_P W - \mathbb{E}_Q W| \leq 2M \|P - Q\|_{TV}.$$

Proof. First note that

$$\mathbb{E}W = \int_0^{2M} \mathbb{P}(W + M \geq t) dt - M.$$

Thus

$$\mathbb{E}_P W - \mathbb{E}_Q W = \int_0^{2M} \mathbb{P}_P(W + M \geq t) - \mathbb{P}_Q(W + M \geq t) dt \leq 2M \|P - Q\|_{TV}.$$

Repeating the argument with P and Q interchanged gives $\mathbb{E}_Q W - \mathbb{E}_P W \leq 2M \|P - Q\|_{TV}$ and hence the result. \square

We now turn to the proof of Proposition 5. By scaling we may assume without loss of generality that $M = 1$. We will frequently use the following fact. Let P_1, P_2 be two probability laws on \mathbb{R}^d and suppose $U \sim P_1$ and $V \sim P_2$. Then for any measurable function $f : \mathbb{R}^d \rightarrow \mathbb{R}^c$, if \tilde{P}_1 and \tilde{P}_2 are the laws of $f(U)$ and $f(V)$ respectively, $\|\tilde{P}_1 - \tilde{P}_2\|_{TV} \leq \|P_1 - P_2\|_{TV}$. It thus suffices to consider the case $d_X = d_Y = d_Z = 1$.

Let $(X, Y, Z) \in \mathbb{R}^3$ is a random triple be a random triple. We define $Q \in \mathcal{Q}_{0,1}$ in the following way: if $(X, Y, Z) \sim Q$, $Z \perp\!\!\!\perp (X, Y)$, $Z \sim U(-1, 1)$, and (X, Y) is uniformly distributed on $(0, 1)^2 \cup (-1, 0)^2$. We note, for later use, that $\mathbb{E}_Q X = \mathbb{E}_Q Y = 0$ and $\mathbb{E}_Q XY = 1/4$.

Next take $P \in \mathcal{P}_{0,M}$ and let functions $f, g : (-1, 1) \rightarrow (-1, 1)$ be defined by $f(z) = \mathbb{E}_P(X|Z = z)$ and $g(z) = \mathbb{E}_P(Y|Z = z)$. Let $\psi : (-1, 1)^3 \rightarrow \mathbb{R}$ be given by

$$\psi(x, y, z) = \{x - f(z)\}\{y - g(z)\}.$$

Note that ψ as $x - f(z), y - g(z) \in (-2, 2)$, ψ takes values in $(-4, 4)$. Also $\mathbb{E}_P \psi(X, Y, Z) = 0$ and $\mathbb{E}_P f(Z)g(Z) = \mathbb{E}_P XY$ as $\mathbb{E}_P(X - f(Z))g(Z) = 0$ and $\mathbb{E}_P f(Z)(Y - g(Z)) = 0$.

Let $\|Q - P\|_{TV} = \delta$. Then

$$\begin{aligned} \mathbb{E}_Q \psi(X, Y, Z) &= \mathbb{E}_Q XY + \mathbb{E}_Q f(Z)g(Z) \\ &\geq 1/4 + \mathbb{E}_P f(Z)g(Z) - 2\delta \\ &= 1/4 + \mathbb{E}_P XY - 2\delta \\ &\geq 1/4 + \mathbb{E}_Q XY - 4\delta = 1/2 - 4\delta, \end{aligned}$$

where we have used Lemma 17 in the second and last lines above. We now apply Lemma 17 once more to give

$$1/2 - 4\delta \leq |\mathbb{E}_Q \psi(X, Y, Z) - \mathbb{E}_P \psi(X, Y, Z)| \leq 8\delta,$$

whence $\delta \geq 1/24$.

C.1.2 Proof of Proposition 16

Proof. Let q_{XYZ} be the density of Q and denote by q_{XY} the marginal density of (X, Y) under Q and similarly for q_X etc. To prove (i), we will consider minimising $\text{KL}(Q||P)$ over distributions $P \in \mathcal{P}_0$. Let \mathcal{P}'_0 be the set of densities of distributions in \mathcal{P}_0 with respect to Lebesgue measure with the added restriction that for $p \in \mathcal{P}'_0$, with a slight abuse of notation we have $\text{KL}(q_{XYZ}||p) < \infty$. The proof will show that \mathcal{P}'_0 is non-empty. Given any $p \in \mathcal{P}'_0$, the conditional independence implies the factorisation $p(x, y, z) = p_1(x|z)p_2(y|z)p_3(z)$, i.e., we can minimise over the individual (conditional) densities p_j , $j \in \{1, 2, 3\}$. Adding and subtracting terms that do not depend on p , we obtain

$$\begin{aligned} & \operatorname{argmin}_{P \in \mathcal{P}_0} \text{KL}(Q||P) \\ &= \operatorname{argmin}_{p \in \mathcal{P}'_0} \left\{ - \int q_{XYZ}(x, y, z) \log p(x, y, z) dx dy dz + \int q_{XYZ}(x, y, z) \log q_{XYZ}(x, y, z) dx dy dz \right\} \\ &= \operatorname{argmin}_{p \in \mathcal{P}'_0} \left\{ - \int q_{XY}(x, y) q_Z(z) \log p_1(x|z) dx dy dz - \int q_{XY}(x, y) q_Z(z) \log p_2(y|z) dx dy dz \right. \\ & \quad \left. - \int q_{XY}(x, y) q_Z(z) \log p_3(z) dx dy dz \right\} \\ &= \operatorname{argmin}_{p \in \mathcal{P}'_0} \left\{ - \int q_X(x) q_Z(z) \log \{p_1(x|z) q_Z(z)\} dx dz - \int q_Y(y) q_Z(z) \log \{p_2(y|z) q_Z(z)\} dy dz \right. \\ & \quad \left. - \int q_Z(z) \log p_3(z) dz \right\}. \end{aligned}$$

Note that the fact that \mathcal{P}'_0 contains only densities p such that $\text{KL}(q_{XYZ}||p) < \infty$ ensures that all of the integrands above are integrable, which permits the use of the additivity property of integrals. From Gibbs' inequality, we know the expression in the last display is minimised by $p_1^*(x|z) = q_X(x)$, $p_2^*(y|z) = q_Y(y)$, and $p_3^*(z) = q_Z(z)$. This implies

$$\inf_{P \in \mathcal{P}_0} \text{KL}(Q||P) = \int q_{XY}(x, y) \log \frac{q_{XY}(x, y)}{q_X(x) q_Y(y)} = I_Q(X; Y) = -\frac{1}{2} \log(1 - \rho_Q^2),$$

where $I_Q(X, Y)$ denotes the mutual information between X and Y , and ρ_Q is the correlation coefficient of the bivariate Gaussian (X, Y) , both under Q .

For the second equality sign, we now minimise $\text{KL}(P||Q)$ with respect to P . Let us redefine \mathcal{P}'_0 to now be the set of densities of distributions in \mathcal{P}_0 with the additional restriction that for $p \in \mathcal{P}'_0$, we have $\text{KL}(p||q_{XYZ}) < \infty$. For such p , we have

$$\text{KL}(p||q_{XYZ}) = \int p_3(z) \int p_1(x|z) p_2(y|z) \log \frac{p_1(x|z) p_2(y|z)}{q_{XY}(x, y)} dx dy dz + \int p_3(z) \log \frac{p_3(z)}{q_Z(z)} dz, \quad (17)$$

again noting that finiteness of $\text{KL}(p||q_{XYZ})$ ensures Fubini's theorem and additivity may be used. We will first consider, for a fixed z , the optimisation over p_1 and p_2 . From variational

Bayes methods we know that

$$\begin{aligned} p_1^*(x|z) &\propto \exp\left(\int_y p_2^*(y|z) \log q_{XYZ}(x, y, z) dy\right) \propto \exp\left(\int_y p_2^*(y|z) \log q_{XY}(x, y) dy\right) \\ p_2^*(y|z) &\propto \exp\left(\int_x p_1^*(x|z) \log q_{XYZ}(x, y, z) dx\right) \propto \exp\left(\int_x p_1^*(x|z) \log q_{XY}(x, y) dx\right). \end{aligned}$$

Straightforward calculations (Section 10.1.2 of Bishop [8]) show that $p_1^*(x|z) = p_1^*(x)$ and $p_2^*(y|z) = p_2^*(y)$ are Gaussian densities with mean zero and variances $\Sigma_{11} := (\Sigma_Q^{-1})_{11}^{-1} = \sigma^2/(\sigma^2 + 1)$ and $\Sigma_{22} := (\Sigma_Q^{-1})_{22}^{-1} = \sigma^2$, respectively, where Σ_Q is the covariance matrix of the bivariate distribution for (X, Y) under Q . It then follows from (17) that $p_3^*(z) = q_Z(z)$. Thus we have,

$$\begin{aligned} \text{KL}(p^*||q_{XYZ}) &= \int p^*(x, y) \log\{p^*(x, y)/q_{XY}(x, y)\} dx dy \\ &= \frac{1}{2} \left(\text{tr}(\Sigma_Q^{-1}\Sigma) - 2 + \log \frac{\det \Sigma_Q}{\det \Sigma} \right) = \frac{1}{2} \log \left(\frac{1 + \sigma^2}{\sigma^2} \right). \end{aligned}$$

□

D Proofs of Results in Section 3

In this section, we will use $a \lesssim b$ as shorthand for $a \leq Cb$ for some constant $C \geq 0$, where what C is constant with respect to will be clear from the context.

D.1 Proof of Theorem 6

First observe that by scaling we may assume without loss of generality that $\mathbb{E}_P((\varepsilon_P \xi_P)^2) = 1$ for all P .

We begin by proving (i). We shall suppress the dependence on P and n at times to lighten the notation. Recall the decomposition,

$$\begin{aligned} \tau_N &= \frac{1}{\sqrt{n}} \sum_{i=1}^n R_i = \frac{1}{\sqrt{n}} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i) + \varepsilon_i\} \{g(z_i) - \hat{g}(z_i) + \xi_i\} \\ &= (b + \nu_f + \nu_g) + \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i \xi_i, \end{aligned} \tag{18}$$

where

$$\begin{aligned} b &:= \frac{1}{\sqrt{n}} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i)\} \{g(z_i) - \hat{g}(z_i)\}, \\ \nu_g &:= \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i \{g(z_i) - \hat{g}(z_i)\}, \quad \nu_f := \frac{1}{\sqrt{n}} \sum_{i=1}^n \xi_i \{f(z_i) - \hat{f}(z_i)\}. \end{aligned}$$

Now

$$\mathbb{E}(\varepsilon_i \xi_i) = \mathbb{E}(\varepsilon_i \xi_i | \mathbf{Y}, \mathbf{Z}) = \xi_i \mathbb{E}(\varepsilon_i | \mathbf{Z}) = 0.$$

Thus the summands $\varepsilon_i \xi_i$ in the final term of (18) are i.i.d. mean zero with finite variance, so the central limit theorem dictates that this converges to a standard normal distribution. By the Cauchy–Schwarz inequality, we have

$$|b| \leq \sqrt{n} A_f^{1/2} B_f^{1/2} \xrightarrow{P} 0. \tag{19}$$

We now turn to ν_f and ν_g . Conditional on \mathbf{Y} and \mathbf{Z} , ν_g is a sum of mean-zero independent terms and

$$\mathbf{var}(\varepsilon_i\{g(z_i) - \hat{g}(z_i)\}|\mathbf{Y}, \mathbf{Z}) = \{g(z_i) - \hat{g}(z_i)\}^2 u(z_i).$$

Thus our condition on B_g gives us that $\mathbb{E}(\nu_g^2|\mathbf{Y}, \mathbf{Z}) \xrightarrow{P} 0$. Thus given $\epsilon > 0$

$$\begin{aligned} \mathbb{P}(\nu_g^2 \geq \epsilon) &= \mathbb{P}(\nu_g^2 \wedge \epsilon \geq \epsilon) \\ &\leq \epsilon^{-1} \mathbb{E}\{\mathbb{E}(\nu_g^2 \wedge \epsilon|\mathbf{Y}, \mathbf{Z})\} \\ &\leq \epsilon^{-1} \mathbb{E}\{\mathbb{E}(\nu_g^2|\mathbf{Y}, \mathbf{Z}) \wedge \epsilon\} \rightarrow 0 \end{aligned} \tag{20}$$

using bounded convergence (Lemma 22).

Using Slutsky's lemma, we may conclude that $\tau_N \xrightarrow{d} \mathcal{N}(0, 1)$. We now argue that the denominator τ_D will converge to 1 in probability, which will give us $T_n \xrightarrow{d} \mathcal{N}(0, 1)$ again by Slutsky's lemma.

First note that from the above we have in particular that $(b + \nu_f + \nu_g)/n \xrightarrow{P} 0$. Thus $\sum_{i=1}^n R_i/n \xrightarrow{P} 0$ by the weak law of large numbers (WLLN). It suffices therefore to show that $\sum_{i=1}^n R_i^2/n \xrightarrow{P} 1$. Now

$$\begin{aligned} |R_i^2 - \varepsilon_i^2 \xi_i^2| &\leq [\{f(z_i) - \hat{f}(z_i)\}^2 + 2|\varepsilon_i\{f(z_i) - \hat{f}(z_i)\}|] [\{g(z_i) - \hat{g}(z_i)\}^2 + 2|\xi_i\{g(z_i) - \hat{g}(z_i)\}|] \\ &\quad + \varepsilon_i^2 [\{g(z_i) - \hat{g}(z_i)\}^2 + 2|\xi_i\{g(z_i) - \hat{g}(z_i)\}|] \\ &\quad + \xi_i^2 [\{f(z_i) - \hat{f}(z_i)\}^2 + 2|\varepsilon_i\{f(z_i) - \hat{f}(z_i)\}|] \\ &= \text{I}_i + \text{II}_i + \text{III}_i. \end{aligned}$$

Multiplying out and using the inequality $2|ab| \leq a^2 + b^2$ we have

$$\begin{aligned} \text{I}_i &\leq 3\{f(z_i) - \hat{f}(z_i)\}^2 \{g(z_i) - \hat{g}(z_i)\}^2 + \varepsilon_i^2 \{g(z_i) - \hat{g}(z_i)\}^2 + \xi_i^2 \{f(z_i) - \hat{f}(z_i)\}^2 \\ &\quad + 4|\varepsilon_i \xi_i \{f(z_i) - \hat{f}(z_i)\} \{g(z_i) - \hat{g}(z_i)\}| \end{aligned}$$

Now

$$\frac{1}{n} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i)\}^2 \{g(z_i) - \hat{g}(z_i)\}^2 \leq n A_f A_g \xrightarrow{P} 0.$$

Next note that for any $\epsilon > 0$,

$$\mathbb{E} \left(\epsilon \wedge \frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \{g(z_i) - \hat{g}(z_i)\}^2 \middle| \mathbf{Y}, \mathbf{Z} \right) = \mathbb{E}(\nu_g^2 \wedge \epsilon | \mathbf{Y}, \mathbf{Z}),$$

so

$$\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \{g(z_i) - \hat{g}(z_i)\}^2 \xrightarrow{P} 0 \tag{21}$$

by the same argument as used to show $\nu_g \xrightarrow{P} 0$. Similarly, we also have that the corresponding term involving f , \hat{f} and ξ_i^2 tends to 0 in probability. For the final term in I_i , we have

$$\frac{1}{n} \sum_{i=1}^n |\varepsilon_i \xi_i \{f(z_i) - \hat{f}(z_i)\} \{g(z_i) - \hat{g}(z_i)\}| \leq \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \xi_i^2 \right)^{1/2} \left(\frac{1}{n} \sum_{i=1}^n \{f(z_i) - \hat{f}(z_i)\}^2 \{g(z_i) - \hat{g}(z_i)\}^2 \right)^{1/2}.$$

The first term above converges to $\{\mathbb{E}(\varepsilon_i^2 \xi_i^2)\}^{1/2}$ by the WLLN and the final term is bounded above by $\sqrt{n A_f A_g} \xrightarrow{P} 0$.

Turning now to Π_i , we have

$$\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 |\xi_i \{g(z_i) - \hat{g}(z_i)\}| \leq \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \xi_i^2 \right)^{1/2} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \{g(z_i) - \hat{g}(z_i)\}^2 \right)^{1/2} \xrightarrow{P} 0$$

by WLLN and (21). Similarly we also have $\sum_{i=1}^n \Pi_i/n \xrightarrow{P} 0$. As $\sum_{i=1}^n \varepsilon_i^2 \xi_i^2/n \xrightarrow{P} \mathbb{E}(\varepsilon_i^2 \xi_i^2) = 1$ by WLLN, we have $\tau_D \xrightarrow{P} 1$ as required.

The uniform result (ii) follows by an analogous argument to the above, the only differences being that all convergence in probability statements must be uniform, and the convergence in distribution via the central limit theorem must also be uniform over \mathcal{P} . These stronger properties follow easily from the stronger assumptions given in the statement of the result; that they suffice for the uniform central limit theorem is shown in Kasy [30].

D.2 Proof of Theorem 8

The proof of this result is very similar to that of Theorem 6, and we will adopt the same notation here. We shall suppress the dependence on P and n at times to lighten the notation. We shall denote the auxiliary dataset by \mathbf{A} . We begin by proving (i). We have

$$\tau_N - \sqrt{n}\rho_P = (b + \nu_f + \nu_g) + \frac{1}{\sqrt{n}} \sum_{i=1}^n (\varepsilon_i \xi_i - \rho). \quad (22)$$

Thus the summands $\varepsilon_i \xi_i - \rho$ in the final term are i.i.d. mean zero with finite variance, so the central limit theorem dictates that this converges to a standard normal distribution.

Control of the term b is identical to that in the proof of Theorem 6. Turning to ν_f and ν_g , Conditional on \mathbf{Z} and the auxiliary dataset \mathbf{A} , ν_g is a sum of mean-zero independent terms and

$$\text{var}(\varepsilon_i \{g(z_i) - \hat{g}(z_i)\} | \mathbf{A}, \mathbf{Z}) = \{g(z_i) - \hat{g}(z_i)\}^2 u(z_i).$$

That $\nu_g \xrightarrow{P} 0$ follows exactly as in the argument preceding (20), and similarly for ν_f . Using Slutsky's lemma, we may conclude that $\tau_N - \sqrt{n}\rho_P \xrightarrow{d} \mathcal{N}(0, 1)$.

The argument that $\tau_D \xrightarrow{P} \sigma$ proceeds similarly to that in the proof of Theorem 6, but with conditioning on \mathbf{X} or \mathbf{Y} replaced by conditioning on \mathbf{A} . The uniform result (ii) follows by an analogous argument, see the comments at the end of the proof of Theorem 6.

D.3 Proof of Theorem 9

The proof of Theorem 9 relies heavily on results from Chernozhukov et al. [14] which we state in the next section for convenience, after which we present the proof Theorem 9.

D.3.1 Results from Chernozhukov et al. [14]

In the following, $W \sim \mathcal{N}_p(0, \Sigma)$ where $\Sigma_{jj} = 1$ for $j = 1, \dots, p$ and $p \geq 3$. Set $V = \max_{j=1, \dots, p} |W_j|$. In addition, let $\tilde{w}_1, \dots, \tilde{w}_n \in \mathbb{R}^p$ be independent random vectors having the same distribution as a random vector \tilde{W} with $\mathbb{E}\tilde{W} = 0$ and covariance matrix Σ .

Consider the following conditions.

$$(B1a) \quad \max_{k=1,2} \mathbb{E}(|\tilde{W}_j|^{2+k}/C_n^k) + \mathbb{E}(\exp(|\tilde{W}_j|/C_n)) \leq 4 \text{ for all } j;$$

$$(B1b) \quad \max_{k=1,2} \mathbb{E}(|\tilde{W}_j|^{2+k}/C_n^{k/2}) + \mathbb{E}(\max_{j=1, \dots, p} |\tilde{W}_j|^4/C_n^2) \leq 4 \text{ for all } j;$$

(B2) $C_n^4(\log(pn))^7/n \leq Cn^{-c}$ for some constants $C, c > 0$.

We will assume that \tilde{W} satisfies one of (B1a) and (B1b), and (B2).

Let

$$\tilde{V} = \max_{j=1,\dots,p} \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n \tilde{w}_{ij} \right|.$$

The labels of the corresponding results in Chernozhukov et al. [14] are given in brackets. A slight difference between our presentation of these results here and the statements in Chernozhukov et al. [14] is that we consider the maximum absolute value rather than the maximum.

Lemma 18 (Lemma 2.1). *There exists a constant $C' > 0$ such that for all $t \geq 0$,*

$$\sup_{w \geq 0} \mathbb{P}(|\max_{j=1,\dots,p} W_j - w| \leq t) \leq C't(\sqrt{2\log(p)} + 1).$$

Theorem 19 (Corollary 2.1). *Then there exists constant $c', C > 0$ such that*

$$\sup_{t \in \mathbb{R}} |\mathbb{P}(\tilde{V} \leq t) - \mathbb{P}(V \leq t)| \lesssim n^{-c}.$$

The following result includes a slight variant of Lemma 3.2 of Chernozhukov et al. [14] whose proof follows in exactly the same way.

Lemma 20 (Lemmas 3.1 and 3.2). *Let $U \in \mathbb{R}^p$ be a centred Gaussian random vector with covariance matrix $\Theta \in \mathbb{R}^{p \times p}$ and let $\Delta_0 = \max_{j,k=1,\dots,p} |\Sigma_{jk} - \Theta_{jk}|$. Define $q(\theta) := \theta^{1/3}(1 \vee \log(p/\theta))^{2/3}$. There exists a constant $C' > 0$ such that the following hold.*

(i)

$$\sup_{t \in \mathbb{R}} |\mathbb{P}(\max_{j=1,\dots,p} U_j \leq t) - \mathbb{P}(V \leq t)| \leq C'q(\Delta_0).$$

(ii) *Writing G_Σ and G_Θ for the quantile functions of W and U respectively,*

$$G_\Theta(\alpha) \leq G_\Sigma(\alpha + C'q(\Delta_0)) \quad \text{and} \quad G_\Sigma(\alpha) \leq G_\Theta(\alpha + C'q(\Delta_0))$$

for all $\alpha \in (0, 1)$.

Lemma 21 (Lemma C.1 and the proof of Corollary 3.1). *Let $\tilde{\Sigma}$ be the empirical covariance matrix formed using $\tilde{w}_1, \dots, \tilde{w}_n$, so $\tilde{\Sigma} = \sum_{i=1}^n \tilde{w}_i \tilde{w}_i^T / n$. Then*

$$\begin{aligned} \log(p)^2 \mathbb{E} \|\tilde{\Sigma} - \Sigma\|_\infty &\lesssim n^{-c'} \\ \log(p)^2 \mathbb{E} \left(\max_{j=1,\dots,p} \left| \frac{1}{n} \sum_{i=1}^n \tilde{w}_{ij} \right| \right) &\lesssim Cn^{-c'}. \end{aligned}$$

for some constants $c' > 0$.

Note the second inequality does not appear in Chernozhukov et al. [14] but follows easily in a similar manner to the first inequality.

D.3.2 Proof of Theorem 9

We will assume, without loss of generality, that $\text{var}_P(\varepsilon_{P,j}\xi_{P,k}) = 1$ for all $P \in \mathcal{P}$. Furthermore, we will suppress dependence on P and n at times in order to lighten the notation. We will use C' to denote a positive constant that may change from line to line.

Note that we have $\mathbb{E}(\varepsilon_j \xi_k) = 0$. Let us decompose $\sqrt{n}\bar{\mathbf{R}}_{jk} = \delta_{jk} + \tilde{T}_{jk}$ where

$$\tilde{T}_{jk} = \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_{ij} \xi_{ik}.$$

Furthermore, let us write the denominator in the definition of T_{jk} as $(\|\mathbf{R}_{jk}\|_2^2/n - \bar{\mathbf{R}}_{jk}^2)^{1/2} = 1 + \Delta_{jk}$. We thus have $T_{jk} = (\tilde{T}_{jk} + \delta_{jk})/(1 + \Delta_{jk})$. Let $\tilde{S}_n = \max_{j,k} |\tilde{T}_{jk}|$.

Let $\mathbf{\Sigma} \in \mathbb{R}^{d_X \cdot d_Y \times d_X \cdot d_Y}$ be the matrix with columns and rows indexed by pairs $jk = (j, k) \in \{1, \dots, d_X\} \times \{1, \dots, d_Y\}$ and entries given by $\Sigma_{jk,lm} = \mathbb{E}(\varepsilon_j \varepsilon_l \xi_k \xi_m)$. Let $W \in \mathbb{R}^{d_X \cdot d_Y}$ be a centred Gaussian random vector with covariance $\mathbf{\Sigma}$ and let V_n be the maximum of the absolute values of components of W . We write G for the quantile function of V_n . Note that from Lemma 18, we have in particular that V_n has no atoms, so $\mathbb{P}(V_n \leq G(\alpha)) = \alpha$ for all $\alpha \in [0, 1]$.

Let

$$\rho_P = \sup_{t \geq 0} |\mathbb{P}_P(S_n \leq t) - \mathbb{P}(V_n \leq t)|.$$

We will first obtain a bound on

$$v_P(\alpha) = |\mathbb{P}_P(S_n \leq \hat{G}(\alpha)) - \alpha|$$

in terms of ρ_P , and later bound ρ_P itself. Fixing $P \in \mathcal{P}$ and suppressing dependence on this, we have

$$\begin{aligned} v(\alpha) &\leq |\mathbb{P}(S_n \leq \hat{G}(\alpha)) - \mathbb{P}(S_n \leq G(\alpha))| + |\mathbb{P}(S_n \leq G(\alpha)) - \mathbb{P}(V_n \leq G(\alpha))| \\ &\leq \mathbb{P}(\{S_n \leq \hat{G}(\alpha)\} \triangle \{S_n \leq G(\alpha)\}) + \rho \end{aligned}$$

where we have used the fact that $|\mathbb{P}(A) - \mathbb{P}(B)| \leq \mathbb{P}(A \triangle B)$. Now from Lemma 20 we know that on the event $\{\|\mathbf{\Sigma} - \hat{\mathbf{\Sigma}}\|_\infty \leq u_\Sigma\}$, we have $G(\alpha - C'q(u_\Sigma)) \leq \hat{G}(\alpha) \leq G(\alpha + C'q(u_\Sigma))$. Thus

$$\begin{aligned} \mathbb{P}(\{S_n \leq \hat{G}(\alpha)\} \triangle \{S_n \leq G(\alpha)\}) &\leq \mathbb{P}\{G(\alpha - C'q(u_\Sigma)) \leq S_n \leq G(\alpha + C'q(u_\Sigma))\} \\ &\leq \mathbb{P}\{S_n \leq G(\alpha + C'q(u_\Sigma))\} + \mathbb{P}(\|\mathbf{\Sigma} - \hat{\mathbf{\Sigma}}\|_\infty > u_\Sigma) \\ &\leq 2\rho + \mathbb{P}\{G(\alpha - C'q(u_\Sigma)) \leq V_n \leq G(\alpha + C'q(u_\Sigma))\} + \mathbb{P}(\|\mathbf{\Sigma} - \hat{\mathbf{\Sigma}}\|_\infty > u_\Sigma) \\ &= 2\rho + 2C'q(u_\Sigma) + \mathbb{P}(\|\mathbf{\Sigma} - \hat{\mathbf{\Sigma}}\|_\infty > u_\Sigma). \end{aligned}$$

This gives

$$v(\alpha) \lesssim \rho + q(u_\Sigma) + \mathbb{P}(\|\mathbf{\Sigma} - \hat{\mathbf{\Sigma}}\|_\infty > u_\Sigma).$$

Now let Ω be the event that $\max_{j,k} |\delta_{jk}| \leq u_\delta$ and $\max_{j,k} |\Delta_{jk}| \leq u_\Delta$.

$$\begin{aligned} \rho &\leq \sup_{t \geq 0} \{|\mathbb{P}(\tilde{S}_n \leq t(1 + u_\Delta) + u_\delta) - \mathbb{P}(V_n \leq t)| + |\mathbb{P}(\tilde{S}_n \leq t(1 - u_\Delta) - u_\delta) - \mathbb{P}(V_n \leq t)|\} + \mathbb{P}(\Omega^c) \\ &\leq \sup_{t \geq 0} \{|\mathbb{P}(\tilde{S}_n \leq t) - \mathbb{P}\{V_n \leq (t - u_\delta)/(1 + u_\Delta)\}| + |\mathbb{P}(\tilde{S}_n \leq t) - \mathbb{P}\{V_n \leq (t + u_\delta)/(1 - u_\Delta)\}|\} + \mathbb{P}(\Omega^c). \end{aligned}$$

Now

$$\begin{aligned} &|\mathbb{P}(\tilde{S}_n \leq t) - \mathbb{P}\{V_n \leq (t - u_\delta)/(1 + u_\Delta)\}| \\ &\leq |\mathbb{P}(\tilde{S}_n \leq t) - \mathbb{P}(V_n \leq t)| + |\mathbb{P}(V_n \leq t - u_\delta) - \mathbb{P}((1 + u_\Delta)V_n \leq t - u_\delta)| + |\mathbb{P}(t - u_\delta \leq V_n \leq t)| \\ &\leq \text{I} + \text{II} + \text{III}. \end{aligned}$$

From Theorem 19, we have $I = o(1)$. Lemma 20 gives

$$II + III \lesssim q(u_\Delta) + u_\delta \sqrt{\log(d_X d_Y)}.$$

Similarly,

$$|\mathbb{P}(\tilde{S}_n \leq t) - \mathbb{P}\{V_n \leq (t + u_\delta)/(1 - u_\Delta)\}| \lesssim q(u_\Delta) + u_\delta \sqrt{\log(d_X d_Y)} + o(1).$$

Putting things together, we have

$$\begin{aligned} v(\alpha) &\lesssim \mathbb{P}(\|\Sigma - \hat{\Sigma}\|_\infty > u_\Sigma) + q(u_\Sigma) + \mathbb{P}(\max_{j,k} |\delta_{jk}| > u_\delta) + u_\delta \sqrt{\log(d_X d_Y)} \\ &\quad + \mathbb{P}(\max_{j,k} |\Delta_{jk}| > u_\Delta) + q(u_\Delta) + o(1). \end{aligned}$$

We thus see that writing $a_n = \log(d_X d_Y)^{-2}$, if $\max_{j,k} |\delta_{jk}| = o_P(a_n^{1/4})$, $\max_{j,k} |\Delta_{jk}| = o_P(a_n)$ and $\|\Sigma - \hat{\Sigma}\|_\infty = o_P(a_n)$, then we will have $\sup_{P \in \mathcal{P}} \sup_{\alpha \in (0,1)} v_P(\alpha) \rightarrow 0$. These remaining properties are shown in Lemma 23.

D.4 Auxiliary Lemmas

Lemma 22. *Let \mathcal{P} be a family of distributions determining the distribution of a sequence of random variables $(W_n)_{n \in \mathbb{N}}$. Suppose $W_n = o_P(1)$ and $|W_n| < C$ for some $C > 0$. Then $\mathbb{E}|W_n| \rightarrow 0$.*

Proof. Given $\epsilon > 0$, there exists N such that $\sup_{P \in \mathcal{P}} \mathbb{P}_P(|W_n| > \epsilon) < \epsilon$ for all $n \geq N$. Thus for such n ,

$$\mathbb{E}_P|W_n| = \mathbb{E}_P(|W_n| \mathbb{1}_{\{|W_n| \leq \epsilon\}}) + \mathbb{E}_P(|W_n| \mathbb{1}_{\{|W_n| > \epsilon\}}) \leq \epsilon + C\epsilon.$$

As ϵ was arbitrary, we have $\sup_{P \in \mathcal{P}} \mathbb{E}_P|W_n| \rightarrow 0$. \square

Lemma 23. *Consider the setup of Theorem 9 and its proof (Section D.3.2). Let $a_n = \log(d_X d_Y)^{-2}$. We have that*

- (i) $\max_{j,k} |\delta_{jk}| = o_P(a_n^{1/4})$;
- (ii) $\max_{j,k} |\Delta_{jk}| = o_P(a_n)$;
- (iii) $\|\Sigma - \hat{\Sigma}\|_\infty = o_P(a_n)$.

Proof. The arguments here are similar to those in the proof of Theorem 6, but with the added complication of requiring uniformity over expressions corresponding to different components of X and Y . We will at times suppress the dependence of quantities on P to lighten notation.

We begin by showing (i). Let us decompose each δ_{jk} as $\delta_{jk} = b_{jk} + \nu_{g,jk} + \nu_{f,jk}$, these terms being defined as the analogues of b , ν_g and ν_f but corresponding to the regression of $\mathbf{X}_j^{(n)}$ and $\mathbf{Y}_j^{(n)}$ on to $\mathbf{Z}^{(n)}$.

By the Cauchy–Schwarz inequality, we have $b_{jk} \leq \sqrt{n} A_{f,j}^{1/2} A_{g,k}^{1/2} = o_P(a_n^{1/4})$ using (6). Let us write $\omega_{ik} = g_k(z_i) - \hat{g}_k(z_i)$. In order to control $\max_{j,k} |\nu_{g,jk}|$ we will use Lemma 26. Given $\epsilon > 0$, we have

$$\mathbb{P}_P(\max_{j,k} |\nu_{g,jk}|/a_n^{1/4} \geq \epsilon) \lesssim \sqrt{\tau \log(d_X d_Y)} \mathbb{E}_P \left\{ \epsilon \wedge \left(\max_k \frac{1}{n a_n^{1/2}} \sum_{i=1}^n \omega_{ik}^2 \right)^{1/4} \right\} + \mathbb{P}_P(\max_{i,j} |\varepsilon_{ij}| > \tau) \quad (23)$$

for all $\tau \geq 0$. As $\max_{i,j} |\varepsilon_{ij}| = O_{\mathcal{P}}(\tau_n)$, we know that given δ , there exists $C > 0$ such that $\sup_{P \in \mathcal{P}} \mathbb{P}_P(\max_{i,j} |\varepsilon_{ij}| > C\tau_{g,n}) < \delta$ for all n . By bounded convergence (Lemma 22) and (8), we then have that

$$\sup_{P \in \mathcal{P}} \sqrt{\tau_{g,n} \log(d_X d_Y)} \mathbb{E}_P \left\{ \epsilon \wedge \left(\max_k \frac{1}{n a_n^{1/2}} \sum_{i=1}^n \omega_{ik}^2 \right)^{1/4} \right\} \rightarrow 0,$$

whence $\max_{j,k} |\nu_{g,jk}| = o_{\mathcal{P}}(a_n^{1/4})$. Similarly $\max_{j,k} |\nu_{f,jk}| = o_{\mathcal{P}}(a_n^{1/4})$, which completes the proof of (i).

Turning to (ii), we see that

$$\max_{j,k} |(1 + \Delta_{jk})^2 - 1| \leq \max_{j,k} \|\mathbf{R}_{jk}\|_2^2/n - 1 + \max_{j,k} |\bar{\mathbf{R}}_{jk}|.$$

Lemma 24 shows that the first term on the RHS is $o_{\mathcal{P}}(a_n)$. For the second term we have

$$\max_{j,k} |\bar{\mathbf{R}}_{jk}| \leq \max_{j,k} |\delta_{jk}|/\sqrt{n} + \max_{j,k} \frac{1}{n} \sum_{i=1}^n \varepsilon_{ij} \xi_{ik} = o_{\mathcal{P}}(a_n)$$

from (i) and Lemma 21, noting that (A2) implies in particular that $\log(d_X d_Y)^3 = o(n)$. Thus applying Lemma 25, we have that $\max_{j,k} |\Delta_{jk}| = o_{\mathcal{P}}(a_n)$.

We now consider (iii). Let $\tilde{\Sigma} \in \mathbb{R}^{d_X d_Y \times d_X d_Y}$ be the matrix with rows and columns indexed by pairs $jk = (j, k) \in \{1, \dots, d_X\} \times \{1, \dots, d_Y\}$ and entries given by

$$\tilde{\Sigma}_{jk,lm} = \frac{1}{n} \sum_{i=1}^n \varepsilon_{ij} \xi_{ik} \varepsilon_{il} \xi_{im}.$$

We know from Lemma 21 that $\|\Sigma - \tilde{\Sigma}\|_{\infty} = o_{\mathcal{P}}(a_n)$. It remains to show that $\|\hat{\Sigma} - \tilde{\Sigma}\|_{\infty} = o_{\mathcal{P}}(a_n)$.

From Lemma 24 we have that

$$\max_{j,k,l,m} |\mathbf{R}_{jk}^T \mathbf{R}_{lm}/n - \bar{\mathbf{R}}_{jk} \bar{\mathbf{R}}_{lm} - \tilde{\Sigma}_{jk,lm}| = o_{\mathcal{P}}(a_n).$$

It suffices to show that

$$\max_{j,k,l,m} |\{(1 + \Delta_{jk})(1 + \Delta_{lm})\}^{-1} - 1| = o_{\mathcal{P}}(a_n). \quad (24)$$

We already know that $\max_{j,k} |\Delta_{jk}| = o_{\mathcal{P}}(a_n)$ so applying Lemma 25, we see that $\max_{j,k} |(1 + \Delta_{jk})^{-1} - 1| = o_{\mathcal{P}}(a_n)$. It is then straightforward to see that (24) holds. This completes the proof of (iii). \square

Lemma 24. *Consider the setup of Theorem 9 and its proof (Section D.3.2) as well as that of Lemma 23. We have that*

$$\max_{j,k,l,m} |\mathbf{R}_{jk}^T \mathbf{R}_{lm}/n - \tilde{\Sigma}_{jk,lm}| = o_{\mathcal{P}}(a_n).$$

Proof. Fix i and consider $R_{jk,i} R_{lm,i} - \varepsilon_{ij} \xi_{ik} \varepsilon_{il} \xi_{im}$. Writing $\eta_j = f_j(z_i) - \hat{f}_j(z_i)$ and $\omega_k = g_k(z_i) - \hat{g}_k(z_i)$, and suppressing dependence on i (so e.g. $\varepsilon_{ij} = \varepsilon_j$) we have

$$\begin{aligned} R_{jk,i} R_{lm,i} - \varepsilon_{ij} \xi_{ik} \varepsilon_{il} \xi_{im} &= (\eta_j + \varepsilon_j)(\omega_k + \xi_k)(\eta_l + \varepsilon_l)(\omega_m + \xi_m) - \varepsilon_j \xi_k \varepsilon_l \xi_m \\ &= \eta_j \omega_k \eta_l \omega_m \\ &\quad + \eta_j \omega_k \eta_l \xi_m + \eta_j \omega_k \omega_m \varepsilon_l + \eta_j \eta_l \omega_m \xi_k + \omega_k \eta_l \omega_m \varepsilon_j \\ &\quad + \eta_j \omega_k \varepsilon_l \xi_m + \eta_j \eta_l \xi_k \xi_m + \eta_j \omega_m \xi_k \varepsilon_l + \omega_k \eta_l \varepsilon_j \xi_m + \omega_k \omega_m \varepsilon_j \varepsilon_l + \eta_l \omega_m \varepsilon_j \xi_k \\ &\quad + \eta_j \xi_k \varepsilon_l \xi_m + \omega_k \varepsilon_j \varepsilon_l \xi_m + \eta_l \varepsilon_j \xi_k \xi_m + \omega_m \varepsilon_j \xi_l \varepsilon_l. \end{aligned}$$

We see that the sum on the RHS contains terms of four different types of which $\eta_j \omega_k \eta_l \omega_m$, $\eta_j \omega_k \eta_l \xi_m$, $\eta_j \omega_k \varepsilon_l \xi_m$ and $\eta_j \xi_k \varepsilon_l \xi_m$ are representative examples. We will control the sizes of each of these when summed up over i . Turning first to $\eta_j \omega_k \eta_l \omega_m$, note that $2|\eta_j \omega_k \eta_l \omega_m| \leq \eta_j^2 \omega_k^2 + \eta_l^2 \omega_m^2$.

The argument of (19) combined with (6) shows that

$$\max_{j,k} \frac{1}{n} \sum_{i=1}^n \eta_{ij}^2 \omega_{ik}^2 = o_{\mathcal{P}}(a_n).$$

Next we have $2|\eta_j \omega_k \eta_l \xi_m| \leq \eta_j^2 \omega_k^2 + \eta_l^2 \xi_m^2$. The argument of (20) combined with (7) shows that

$$\max_{l,m} \frac{1}{n} \sum_{i=1}^n \eta_{il}^2 \xi_{im}^2 = o_{\mathcal{P}}(a_n^2) = o_{\mathcal{P}}(a_n).$$

Considering the third term, we have $2|\eta_j \omega_k \varepsilon_l \xi_m| \leq \eta_j^2 \xi_m^2 + \omega_k^2 \varepsilon_l^2$, so this term is also controlled in the same way.

Finally, turning to the fourth term,

$$\begin{aligned} \max_{j,k,l,m} \frac{1}{n} \left| \sum_{i=1}^n \eta_{ij} \xi_{ik} \varepsilon_{il} \xi_{im} \right| &\leq \max_{l,m} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_{il}^2 \xi_{im}^2 \right)^{1/2} \max_{j,k} \left(\frac{1}{n} \sum_{i=1}^n \eta_{ij}^2 \xi_{ik}^2 \right)^{1/2} \\ &= O_{\mathcal{P}}(1) o_{\mathcal{P}}(a_n) = o_{\mathcal{P}}(a_n). \end{aligned}$$

This completes the proof of the result. \square

Lemma 25. *Let \mathcal{P} be a family of distributions determining the distribution of a triangular array of random variables $W^{(n)} \in \mathbb{R}^{p_n}$. Suppose that for some sequence $(a_n)_{n \in \mathbb{N}}$, $\max_{j=1, \dots, p_n} W_j^{(n)} = o_{\mathcal{P}}(a_n)$ as $n \rightarrow \infty$. Then if $D \subset \mathbb{R}$ contains an open neighbourhood of 0 and the function $f : D \rightarrow \mathbb{R}$ is continuously differentiable at 0 with $f(0) = c$, we have*

$$\max_{j=1, \dots, p_n} \{f(W_j^{(n)}) - c\} = o_{\mathcal{P}}(a_n).$$

Proof. Let $\epsilon, \delta > 0$. As f' is continuous at 0, it is bounded on a sufficiently small interval $(-\delta', \delta') \subseteq D$. Let $M = \sup_{x \in (-\delta', \delta')} |f'(x)|$ and set $\eta = \min(\delta', \delta/M)$. Note by the mean-value theorem we have the inequality $|f(x) - c| \leq M|x| \leq \delta$ for all $x \in (-\eta, \eta)$. Thus

$$a_n \max_j |f(W_j^{(n)}) - c| > \delta \subseteq a_n \max_j |W_j^{(n)}| > \eta.$$

Now we have that there exists N such that for all $n \geq N$, $\mathbb{P}_P(a_n \max_j |W_j^{(n)}| > \eta) < \epsilon$ for all $P \in \mathcal{P}$, so from the display above we have that for such n , $\mathbb{P}_P(a_n \max_j |f(W_j^{(n)}) - c| > \delta) < \epsilon$. \square

Lemma 26. *Let $W \in \mathbb{R}^{n \times d_W}$, $V \in \mathbb{R}^{n \times d_V}$ be random matrices such that $\mathbb{E}(W|V) = 0$ and the rows of W are independent conditional on V . Then for $\epsilon > 0$*

$$\epsilon \mathbb{P} \left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n W_{ij} V_{ij} \right| > \epsilon \right) \lesssim \sqrt{\lambda \log(p)} \mathbb{E} \left\{ \epsilon \wedge \left(\max_j \frac{1}{n} \sum_{i=1}^n V_{ij}^2 \right)^{1/4} \right\} + \epsilon \mathbb{P}(\|W\|_{\infty} > \lambda)$$

for any $\lambda \geq 0$.

Proof. We have from Markov's inequality

$$\epsilon \mathbb{P}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n W_{ij} V_{ij} \right| > \epsilon\right) \leq \mathbb{E}\left\{\mathbb{E}\left(\epsilon \wedge \max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n W_{ij} V_{ij} \right| \middle| V\right)\right\}.$$

We will apply a symmetrisation argument to the inner conditional expectation. To this end, introduce W' such that W' and W have the same distribution conditional on V and such that $W' \perp\!\!\!\perp W|V$. In addition, let S_1, \dots, S_n be i.i.d. Rademacher random variables independent of all other quantities. The RHS of the last display is equal to

$$\begin{aligned} & \mathbb{E}\left\{\mathbb{E}\left(\epsilon \wedge \max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n (W_{ij} - \mathbb{E}(W'_{ij}|W, V)) V_{ij} \right| \middle| V\right)\right\} \\ & \leq \mathbb{E}\left[\mathbb{E}\left\{\epsilon \wedge \mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n (W_{ij} - W'_{ij}) V_{ij} \right| \middle| V, W\right) \middle| V\right\}\right] \\ & \leq \mathbb{E}\left\{\epsilon \wedge \mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n (W_{ij} - W'_{ij}) V_{ij} \right| \middle| V\right)\right\} \\ & = \mathbb{E}\left\{\epsilon \wedge \mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n S_i (W_{ij} - W'_{ij}) V_{ij} \right| \middle| V\right)\right\} \\ & \leq 2\mathbb{E}\left\{\epsilon \wedge \mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n S_i W_{ij} V_{ij} \right| \middle| V\right)\right\} \end{aligned}$$

using the triangle inequality in the final line. Now fixing a $\lambda \geq 0$, define $\tilde{W}_{ij} = W_{ij} \mathbb{1}_{\{\|W\|_\infty \leq \lambda\}}$. Half the final expression in the display above is at most

$$\mathbb{E}\left\{\epsilon \wedge \mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n S_i \tilde{W}_{ij} V_{ij} \right| \middle| V\right)\right\} + \epsilon \mathbb{P}(\|W\|_\infty > \lambda).$$

Note that $S_i \tilde{W}_{ij} \in [-\lambda, \lambda]$ and conditional on V , $\{S_i \tilde{W}_{ij}\}_{i=1}^n$ are independent. Thus conditional on V , $\sum_{i=1}^n S_i \tilde{W}_{ij} V_{ij} / \sqrt{n}$ is sub-Gaussian with parameter $\lambda \left(\sum_{i=1}^n V_{ij}^2 / n\right)^{1/2}$. Using a standard maximal inequality for sub-Gaussian random variables (see Theorem 2.5 in Boucheron et al. [9]), we have

$$\mathbb{E}\left(\max_j \left| \frac{1}{\sqrt{n}} \sum_{i=1}^n S_i \tilde{W}_{ij} V_{ij} \right| \middle| V\right) \leq \sqrt{2\lambda \log(p)} \max_j \left(\sum_{i=1}^n V_{ij}^2 / n\right)^{1/4}$$

which then gives the result. \square

E Proof of Theorem 11

We will prove (ii) first. From Theorem 6 and Remark 7, it is enough to show that

$$\sup_{P \in \mathcal{P}} \mathbb{E}_P \left(\frac{1}{n} \sum_{i=1}^n \{f_P(z_i) - \hat{f}(z_i)\}^2 \right) = o(\sqrt{n}), \quad (25)$$

and an analogous result for \hat{g} . We know from Lemma 27 that

$$\frac{1}{n} \sum_{i=1}^n \mathbb{E}_P [\{f_P(z_i) - \hat{f}(z_i)\}^2 | \mathbf{Z}^{(n)}] \leq \max(\sigma^2, \|f_P\|_{\mathcal{H}}^2) \inf_{\lambda > 0} \left\{ \frac{1}{n\lambda} \sum_{i=1}^n \min(\hat{\mu}_i/4, \lambda) + \lambda/4 \right\}.$$

Lemma 28 then gives us

$$\begin{aligned}\mathbb{E}_P \min_{\lambda > 0} \left\{ \frac{1}{n\lambda} \sum_{i=1}^n \min(\hat{\mu}_i/4, \lambda) + \lambda/4 \right\} &\leq \inf_{\lambda > 0} \left\{ \frac{1}{n\lambda} \sum_{i=1}^n \mathbb{E}_P \min(\hat{\mu}_i/4, \lambda) + \lambda/4 \right\} \\ &\leq \inf_{\lambda > 0} \left\{ \frac{C}{n\lambda} \sum_{j=1}^{\infty} \min(\mu_{P,j}, \lambda) + \lambda \right\}\end{aligned}$$

for a constant $C > 0$. Note that the first inequality in the last display allows us to effectively move from a fixed design with a design-dependent tuning parameter λ to a random design but where λ is fixed since the minimum is outside the expectation. For $P \in \mathcal{P}$, let $\phi_P : [0, \infty) \rightarrow [0, \infty)$ be given by

$$\phi_P(\lambda) = \sum_{j=1}^{\infty} \min(\mu_{P,j}, \lambda).$$

Observe that ϕ_P is increasing and $\lim_{\lambda \downarrow 0} \sup_{P \in \mathcal{P}} \phi_P(\lambda) = 0$ by (11). Let $\lambda_{P,n} = n^{-1/2} \sqrt{\phi_P(n^{-1/2})}$ so $\sup_{P \in \mathcal{P}} \lambda_{P,n} = o(n^{-1/2})$. Thus for n sufficiently large $\phi_P(\lambda_{P,n}) \leq \phi_P(n^{-1/2})$, whence for such n we have

$$\begin{aligned}\sup_{P \in \mathcal{P}} \inf_{\lambda > 0} \{ \phi_P(\lambda)/(n\lambda) + \lambda \} &\leq \sup_{P \in \mathcal{P}} \frac{\phi_P(\lambda_{P,n})}{n\lambda_{P,n}} + \lambda_{P,n} \\ &\leq \sup_{P \in \mathcal{P}} \sqrt{\phi_P(n^{-1/2})}/\sqrt{n} = o(n^{-1/2}).\end{aligned}$$

Putting things together gives (25).

To show (i), set $\mathcal{P} = \{P\}$ in the preceding argument and note that $\lim_{\lambda \downarrow 0} \phi_P(\lambda) = 0$ by dominated convergence theorem from the summability of the eigenvalues i.e. (11) always holds.

E.1 Auxiliary Lemmas

The following result gives a bound on the prediction error of kernel ridge regression with fixed design. The arguments are similar to those used in the analysis of regular ridge regression, see for example Dhillon et al. [18].

Lemma 27. *Let $z_1, \dots, z_n \in \mathcal{Z}$ be deterministic and suppose*

$$x_i = f(z_i) + \varepsilon_i$$

where $\text{var}(\varepsilon_i) \leq \sigma^2$, $\text{cov}(\varepsilon_i, \varepsilon_j) = 0$ for $j \neq i$ and $f \in \mathcal{H}$ for some RKHS $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ with reproducing kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$. Consider performing kernel ridge regression with tuning parameter $\lambda > 0$:

$$\hat{f}_{\lambda} = \operatorname{argmin}_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \{x_i - h(z_i)\}^2 + \lambda \|f\|_{\mathcal{H}}^2 \right\}.$$

Let $K \in \mathbb{R}^{n \times n}$ have ij th entry $K_{ij} = k(z_i, z_j)/n$ and denote the eigenvalues of K by $\hat{\mu}_1 \geq \hat{\mu}_2 \geq \dots \geq \hat{\mu}_n \geq 0$. Then we have

$$\begin{aligned}\frac{1}{n} \mathbb{E} \left\{ \sum_{i=1}^n \{f(z_i) - \hat{f}_{\lambda}(z_i)\}^2 \right\} &\leq \frac{\sigma^2}{n} \sum_{i=1}^n \frac{\hat{\mu}_i^2}{(\hat{\mu}_i + \lambda)^2} + \|f\|_{\mathcal{H}}^2 \frac{\lambda}{4} \\ &\leq \frac{\sigma^2}{\lambda} \frac{1}{n} \sum_{i=1}^n \min(\hat{\mu}_i/4, \lambda) + \|f\|_{\mathcal{H}}^2 \frac{\lambda}{4}.\end{aligned}\tag{26}$$

Proof. Let $\mathbf{X} = (x_1, \dots, x_n)^T$. We know from the representer theorem [32, 50] that

$$\left(\hat{f}_\lambda(z_1), \dots, \hat{f}_\lambda(z_n)\right)^T = K(K + \lambda I)^{-1} \mathbf{X}.$$

We now show that

$$\left(f(z_1), \dots, f(z_n)\right)^T = K\alpha,$$

for some $\alpha \in \mathbb{R}^n$, and moreover that $\|f\|_{\mathcal{H}}^2 \geq \alpha^T K \alpha / n$.

Let $V = \text{span}\{k(\cdot, z_1), \dots, k(\cdot, z_n)\} \subseteq \mathcal{H}$ and write $f = u + v$ where $u \in V$ and $v \in V^\perp$. Then

$$f(z_i) = \langle f, k(\cdot, z_i) \rangle = \langle u, k(\cdot, z_i) \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product of \mathcal{H} . Write $u = \sum_{i=1}^n \alpha_i k(\cdot, z_i)$. Then

$$f(z_i) = \sum_{j=1}^n \alpha_j \langle k(\cdot, z_j), k(\cdot, z_i) \rangle = \sum_{j=1}^n \alpha_j k(z_j, z_i) = K_i^T \alpha,$$

where K_i is the i th column (or row) of K . Thus $K\alpha = \left(f(z_1), \dots, f(z_n)\right)^T$. By Pythagoras' theorem

$$\|f\|_{\mathcal{H}}^2 = \|u\|_{\mathcal{H}}^2 + \|v\|_{\mathcal{H}}^2 \geq \|u\|_{\mathcal{H}}^2 = \alpha^T K \alpha / n.$$

Now let the eigendecomposition of K be given by $K = UDU^T$ with $D_{ii} = \hat{\mu}_i$ and define $\theta = U^T K \alpha$. We see that n times the left-hand side of (26) is

$$\begin{aligned} \mathbb{E} \|K(K + \lambda I)^{-1}(U\theta + \varepsilon) - U\theta\|_2^2 &= \mathbb{E} \|DU^T(UDU^T + \lambda I)^{-1}(U\theta + \varepsilon) - \theta\|_2^2 \\ &= \mathbb{E} \|D(D + \lambda I)^{-1}(\theta + U^T \varepsilon) - \theta\|_2^2 \\ &= \mathbb{E} \|\{D(D + \lambda I)^{-1} - I\}\theta\|_2^2 + \mathbb{E} \|D(D + \lambda I)^{-1}U^T \varepsilon\|_2^2. \end{aligned}$$

Let $\Sigma \in \mathbb{R}^{n \times n}$ be the diagonal matrix with i th diagonal entry $\text{var}(\varepsilon_i) \leq \sigma^2$. To compute the second term, we argue as follows.

$$\begin{aligned} \mathbb{E} \|D(D + \lambda I)^{-1}U^T \varepsilon\|_2^2 &= \mathbb{E} [\{D(D + \lambda I)^{-1}U^T \varepsilon\}^T D(D + \lambda I)^{-1}U^T \varepsilon] \\ &= \mathbb{E} [\text{tr}\{D(D + \lambda I)^{-1}U^T \varepsilon \varepsilon^T U D(D + \lambda I)^{-1}\}] \\ &= \text{tr}\{D(D + \lambda I)^{-1}U^T \Sigma U D(D + \lambda I)^{-1}\} \\ &= \text{tr}\{UD^2(D + \lambda I)^{-2}U^T \Sigma\} \\ &\leq \sigma^2 \text{tr}\{D^2(D + \lambda I)^{-2}\} \\ &= \sigma^2 \sum_{i=1}^n \frac{\hat{\mu}_i^2}{(\hat{\mu}_i + \lambda)^2}. \end{aligned}$$

For the first term, we have

$$\|\{D(D + \lambda I)^{-1} - I\}\theta\|_2^2 = \sum_{i=1}^n \frac{\lambda^2 \theta_i^2}{(\hat{\mu}_i + \lambda)^2}.$$

Now as $\theta = DU^T \alpha$ note that $\theta_i = 0$ when $d_i = 0$. Let D^+ be the diagonal matrix with i th diagonal entry equal to D_{ii}^{-1} if $D_{ii} > 0$ and 0 otherwise. Then

$$\sum_{i: \hat{\mu}_i > 0} \frac{\theta_i^2}{\hat{\mu}_i} = \|\sqrt{D^+} \theta\|_2^2 = \alpha^T K U D^+ U^T K \alpha = \alpha^T U D D^+ D U^T \alpha = \alpha^T K \alpha \leq n \|f\|_{\mathcal{H}}^2.$$

Next

$$\sum_{i=1}^n \frac{\theta_i^2}{\hat{\mu}_i} \frac{\hat{\mu}_i \lambda^2}{(\hat{\mu}_i + \lambda)^2} \leq n \|f\|_{\mathcal{H}}^2 \max_{i=1, \dots, n} \frac{\hat{\mu}_i \lambda^2}{(\hat{\mu}_i + \lambda)^2} \leq \lambda n \|f\|_{\mathcal{H}}^2 / 4,$$

using the inequality $(a + b)^2 \geq 4ab$ in the final line. Finally note that

$$\frac{\hat{\mu}_i^2}{(\hat{\mu}_i + \lambda)^2} \leq \min\{1, \hat{\mu}_i^2 / (4\hat{\mu}_i \lambda)\} = \min(\lambda, \hat{\mu}_i / 4) / \lambda.$$

Putting things together gives the result. \square

The following result is an immediate consequence of Propositions 3.3 and 3.4 of Koltchinskii [34].

Lemma 28. *Consider the setup of Theorem 11. There exists an absolute constant $C > 0$ such that for all $r > 0$,*

$$\mathbb{E} \left(\frac{1}{n} \sum_{i=1}^n \min(\hat{\mu}_i / 4, r) \right) \leq \frac{C}{n} \sum_{i=1}^{\infty} \min(\mu_i / 4, r).$$

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