# A Consistent ICM-based $\chi^2$ Specification Test

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May 17, 2024

First Draft: August 30, 2022

#### Abstract

In spite of the omnibus property of Integrated Conditional Moment (ICM) specification tests, they are not commonly used in empirical practice owing to, e.g., the non-pivotality of the test and the high computational cost of available bootstrap schemes especially in large samples. This paper proposes specification and mean independence tests based on a class of ICM metrics termed the generalized martingale difference divergence (GMDD). The proposed tests exhibit consistency, asymptotic  $\chi^2$ distribution under the null hypothesis, and computational efficiency. Moreover, they demonstrate robustness to heteroskedasticity of unknown form and can be adapted to enhance power towards specific alternatives. A power comparison with classical bootstrap-based ICM tests using Bahadur slopes is also provided. Monte Carlo simulations are conducted to showcase the proposed tests' excellent size control and competitive power.

Keywords: specification test, mean independence, martingale difference divergence, omnibus, pivotal

JEL classification: C12, C21, C52

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### 1 Introduction

Model misspecification is a major source of misleading inference in empirical work. This issue is further compounded when various competing models are available. It is thus imperative that modelbased statistical inference be accompanied by proper model checks such as specification tests (Stute, 1997).

Existing tests in the specification testing literature can be categorized into three classes, namely, conditional moment (CM) tests, non-parametric tests, and integrated conditional moment (ICM) tests. The class of CM tests, such as those proposed by Newey (1985) and Tauchen (1985), is not consistent as it relies on only a finite number of moment conditions implied by the null hypothesis (Bierens, 1990). The class of non-parametric tests is therefore proposed as a remedy, see e.g. Fan and Li (2000), Hardle and Mammen (1993), Hong and White (1995), Li et al. (2022), Li and Wang (1998), Su and White (2007), Wooldridge (1992), Yatchew (1992), and Zheng (1996). The key idea is to use an approximately infinite number of moment conditions, a characteristic that often necessitates user-defined parameters such as bandwidths or the number of sieves.

The class of non-parametric tests may encounter challenges such as non-parametric smoothing and suboptimal performance stemming from over-fitting the non-parametric alternative. On the other hand, the class of ICM tests, such as those introduced by Antoine and Lavergne (2022), Bierens (1982, 1990), Bierens and Ploberger (1997), Delgado (1993), Delgado et al. (2006), Domínguez and Lobato (2015), Escanciano (2006a), Stute (1997), and Su and Zheng (2017), has gained popularity due to its ability to avoid these issues and detect local alternatives at faster rates. ICM metrics, on which ICM tests are based, also appear in other contexts: martingale difference hypothesis tests (Escanciano, 2009), joint coefficient and specification tests (Antoine & Lavergne, 2022), model-free feature screening (Li et al., 2023; Shao & Zhang, 2014; Zhu et al., 2011), model estimation (Escanciano, 2018; Tsyawo, 2023), specification tests of the propensity score (Sant'Anna & Song, 2019), and tests of the instrumental variable (IV) relevance condition in ICM estimators (Escanciano, 2018; Tsyawo, 2023).

Despite their advantages, ICM tests are not widely used in empirical research (Domínguez & Lobato, 2015). First, ICM test statistics are not pivotal under the null hypothesis, thus critical values cannot

be tabulated analytically (Bierens & Ploberger, 1997; Domínguez & Lobato, 2015). Second, ICM tests, as commonly implemented, incur a high computational cost due to a large number of bootstrap samples needed to compute *p*-values. Third, although ICM tests are omnibus (Bierens, 1982; Domínguez & Lobato, 2015; Stute, 1997), they only have substantial local power against alternatives in a finite-dimensional space (Escanciano, 2009). Moreover, it is not obvious how to leverage prior knowledge of potential directions under the alternative in order to enhance the power of ICM tests.

In light of the foregoing, this paper proposes consistent  $\chi^2$ -tests of mean independence and model specification. The statistical foundation of our tests rests on a class of newly developed ICM metrics called generalized martingale difference divergence (GMDD) in Li et al. (2023). As a generalization of the martingale difference divergence ICM metric proposed by (Shao & Zhang, 2014), GMDD inherits the advantages of ICM metrics and goes further by providing researchers with a wider array of choices of ICM metrics derived from both integrable and non-integrable integrating measures. Furthermore, the GMDD framework explicitly allows for endogenous regressors, instrumental variables (IV), and heteroskedasticity of unknown form in both linear and non-linear models. Therefore, our tests are ICM-based and omnibus, suggesting their capability to detect all forms of model misspecification including those that violate IV exogeneity conditions.

Compared to existing ICM tests, our tests are more advantageous in three aspects. First, they can be implemented as a  $\chi^2$ - or two-sided *t*-test, which can be interpreted more easily when compared to bootstrap-based tests. Second, the tests do not require bootstrap calibration of critical values, and hence are computationally fast and remain feasible even in very large samples. Third, although our proposed tests are not optimal, their power can be enhanced with the knowledge of directions under the alternative or more generally, with directions the researcher may have in mind whereas ICM tests lack this property. Therefore, we consider our tests as a bridge between CM tests and ICM tests. However, we acknowledge a drawback of our approach, namely, the requirement of a tuning parameter when computing the generalized inverse in forming the Wald-type test statistics.

This paper is not the first attempt at circumventing the non-pivotality of ICM test statistics. Bierens (1982) approximates the critical values of the ICM specification test using Chebyshev's inequality for

first moments under the null hypothesis, which is subsequently improved upon by Bierens and Ploberger (1997). Bierens (1982) also proposes a  $\chi^2$ -test based on two estimates of Fourier coefficients and a carefully chosen tuning parameter. Simulation evidence therein shows a high level of sensitivity to the tuning parameter. Besides, estimating Fourier coefficients no longer makes the test ICM as the test statistic is no longer "integrated". Another attempt in the literature is the conditional Monte Carlo approach of De Jong (1996) and Hansen (1996). These are, however, computationally costly as Bierens and Ploberger (1997) notes.

The rest of the paper is organized as follows. Section 2 provides a brief literature review of ICM metrics and provides background information on the GMDD. Section 3 reformulates the hypothesis test of mean independence, proposes a new charaterization, and establishes its omnibus property. Section 4 proposes the test statistic and derives the asymptotic distribution under the null, local, and alternative hypotheses. Section 5 extends the test of mean independence to model specification. Monte Carlo simulations in Section 6 compare the empirical size and power of the  $\chi^2$  specification test to bootstrapbased ICM specification tests, and Section 7 concludes. All technical proofs and additional simulation results are relegated to the supplementary material.

**Notation:** For  $a \in \mathbb{R}^p$ , we denote its transpose by  $a^{\top}$ , and its Euclidean norm as ||a||. For  $a, b \in \mathbb{R}$ , we denote  $a \wedge b = \min\{a, b\}$ . We denote i as the imaginary unit which satisfies  $i^2 = -1$ . " $\stackrel{p}{\rightarrow}$ " and " $\stackrel{d}{\rightarrow}$ " denote convergence in probability and distribution, respectively. Throughout the paper, for a random vector W, we denote  $W^{\dagger}$  as its independent and identically distributed (*iid*) copy, and write  $\mathbb{E}_n W = n^{-1} \sum_{i=1}^n W_i$  as the empirical mean for *iid* copies  $\{W_i\}_{i=1}^n$  of W. To cut down on notational clutter,  $\widetilde{W}$  is sometimes used to denote the centered version of a random variable W, i.e.,  $\widetilde{W} := W - \mathbb{E}W$ .

# 2 Integrated Conditional Moment Metrics

In this section, we briefly review recent developments in the literature on ICM metrics and provide some background to the concept of GMDD and its use in quantifying mean dependence. For a random variable  $U \in \mathbb{R}$  and a random vector  $Z \in \mathbb{R}^{p_z}$ , we say U is mean-independent of Z, if

$$\mathbb{E}[U|Z] = \mathbb{E}[U] \ almost \ surely \ (a.s.), \tag{1}$$

otherwise, U is mean-dependent on Z.

### 2.1 A Literature Review of ICM metrics

To characterize the relationship (1), the existing literature puts much effort into studying ICM mean dependence metrics of the form:

$$T(U|Z;\nu) = \int_{\Pi} \left| \mathbb{E}[(U - \mathbb{E}U)w(s,Z)] \right|^2 \nu(ds)$$
<sup>(2)</sup>

where w(s, Z) is a weight function, the index s is defined on an appropriate space  $\Pi$ , and  $\nu(\cdot)$  is a suitable integrating measure on  $\Pi$ .

A notable feature of  $T(U|Z;\nu)$  is its omnibus property, namely,  $T(U|Z;\nu) = 0$  if and only if (1) holds, see e.g., Shao and Zhang (2014, Theorem 1.2). The omnibus property guarantees the consistency of ICM tests. Therefore, a larger value of  $T(U|Z;\nu)$  indicates a stronger mean dependence of U on Z. Examples of weight functions from the literature include the step function  $w(s, Z) = I(Z \leq s)$ , e.g., Delgado et al. (2006), Domínguez and Lobato (2004), Escanciano (2006b), Stute (1997), and Zhu et al. (2011); a onedimensional projection in the step function  $w(s, Z) = I(Z^{\top}s_{-1} \leq s_1)$ , e.g., Escanciano (2006a) and Kim et al. (2020); the real exponential  $w(s, Z) = \exp(Z^{\top}s)$ , e.g., Bierens (1990); and the complex exponential  $w(s, Z) = \exp(iZ^{\top}s)$ , e.g., Antoine and Lavergne (2022), Bierens (1982), and Shao and Zhang (2014). The space  $\Pi$  in Escanciano (2006a) and Kim et al. (2020) is given by  $\Pi = \mathbb{R} \times \mathbb{S}_{p_z}$  where  $\mathbb{S}_{p_z}$  denotes the space of  $p_z \times 1$  vectors with unit Euclidean norm while  $\Pi = \mathbb{R}^{p_z}$  for the other works mentioned above. See Escanciano (2006b, Lemma 1) for a general characterization of ICM weight functions. The real and complex exponential functions belong to a larger class of generically comprehensively revealing (GCR) functions, see (Bierens & Ploberger, 1997; Stinchcombe & White, 1998). Other GCR functions include  $w(s, Z) = \sin(Z^{\top}s), w(s, Z) = \sin(Z^{\top}s) + \cos(Z^{\top}s),$  and  $w(s, Z) = 1/(1 + \exp(c - Z^{\top}s)), c \neq 0$ , see Stinchcombe and White (1998) for a discussion.

The choices of w(s, Z) and  $\nu$  are important for practical purposes. First, different choices of w(s, Z)and  $\nu$  result in different  $T(U|Z;\nu)$  that may have varying degrees of sensitivity to the dimension of Z, see, e.g. Escanciano (2006a) and Tsyawo (2023). Second, without a careful choice of weight function and integrating measure, one may need to have recourse to numerical integration in  $T(U|Z;\nu)$ , which is inconvenient in practice (Bierens & Wang, 2012). This paper focuses on the specific choice of the complex exponential weight function  $w(s,Z) = \exp(iZ^{\top}s)$  while allowing for a vast array of (possibly non-integrable) integrating measures  $\nu(\cdot)$ .

### 2.2 Generalized Martingale Difference Divergence

GMDD was originally presented as a byproduct of this paper, but shortly after the first draft was finished, we noticed that the same idea has been independently proposed by Li et al. (2023). To save space, we only provide necessary concepts of the GMDD here and refer the interested reader to Section S.3 in the supplement and Li et al. (2023).

**Definition 2.1** (GMDD). Let  $\nu(\cdot)$  be symmetric about the origin.

$$\mathrm{GMDD}(U|Z) = \int_{\mathbb{R}^{p_z}} \left| \mathbb{E}[(U - \mathbb{E}[U]) \exp(\mathrm{i} Z^{\top} s)] \right|^2 \nu(ds)$$

is called generalized martingale difference divergence (GMDD), if either of the following conditions is satisfied:

- (i)  $\nu$  is an integrable measure on  $\mathbb{R}^{p_z}$ ;
- (ii) for some  $\alpha \in (0,2)$ ,  $\int_{\mathbb{R}^{p_z}} 1 \wedge ||s||^{\alpha} \nu(ds) < \infty$  with  $\mathbb{E}|U|^2 + \mathbb{E}||Z||^{\alpha} < \infty$ .

We note that GMDD in Definition 2.1 is more general than that of Li et al. (2023), where they require that condition (ii) hold with  $\alpha = 2$  under the special choice of the Lévy measure, see equation (1) and the ensuing discussion therein. Clearly, the GMDD is a subclass of ICM metrics, and therefore has the following omnibus property:

$$GMDD(U|Z) = 0 \quad \text{if and only if} \quad \mathbb{E}[U|Z] = \mathbb{E}[U] \ almost \ surely \ (a.s). \tag{3}$$

By (2) and (3), GMDD(U|Z) > 0 if and only if  $\mathbb{E}[U|Z] \neq \mathbb{E}[U]$  a.s. This is the property exploited in ICM tests by transforming the mean independence condition (1) into an equivalent expression based on a scalar-valued GMDD metric. It can shown that (see Proposition S.3.2 in the supplement) if  $\mathbb{E}[U^2 + K^2(Z)] < \infty$ , then

$$GMDD(U|Z) = -\mathbb{E}[(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)K(Z - Z^{\dagger})],$$

where  $K(x) := \int_{\mathbb{R}^{p_z}} (1 - \cos(s^\top x))\nu(ds)$ . Multiple choices of the kernel  $K(\cdot)$  are possible. For example, one can choose  $\nu(\cdot)$  to be density functions of generalized normal distributions so that  $K(z) = -\exp(-||z||^{\alpha}), \alpha > 0$  with special cases of  $\alpha = 1$  and  $\alpha = 2$  corresponding to the Laplacian and Gaussian kernels, respectively, which are commonly used in the machine learning community. One can also choose K(z) = ||z|| which yields the MDD in Shao and Zhang (2014). See Section S.3.2 in the supplement for more examples. Compared with general ICM metrics, the main advantage of using the GMDD is that the integral in (2) can be obtained analytically, which greatly reduces the computational cost due to numerical integration.

**Remark 2.1.** The purpose of Definition 2.1 is to offer practitioners a range of integrating measures (and corresponding kernels). Practitioners concerned about the potential restrictiveness of the moment condition  $\mathbb{E}||Z||^{\alpha} < \infty$  can opt for Laplacian or Gaussian integrating kernels which are bounded. Additionally, since  $\alpha$  can be selected from the interval (0,2), practitioners worried about possible moment condition failures can simply choose a small  $\alpha$ , such as  $\alpha = 0.5$  so that only fractional moments are required for Z. Moreover, considering the possibility of replacing (or redefining) Z with its element-wise bounded one-to-one mapping such that Z and its mapping generate the same Euclidean Borel field—e.g.,  $\operatorname{atan}(Z)$ —as discussed in Bierens (1982, 1982, p. 108), the moment restrictions are practically mild. In practice, we consider the following empirical estimator of GMDD(U|Z), namely

$$\operatorname{GMDD}_{n}(U|Z) = -\frac{1}{n(n-1)} \sum_{i \neq j} (U_{i} - \mathbb{E}_{n}[U])(U_{j} - \mathbb{E}_{n}[U])K(Z_{i} - Z_{j}).$$

$$\tag{4}$$

Like most existing tests based on ICM metrics, the asymptotic null distribution (under (1)) of the empirical estimator of GMDD is non-pivotal.

**Proposition 2.1.** Let  $\mathbb{E}[U^2 U^{\dagger 2} K^2 (Z - Z^{\dagger})] < \infty$  hold.

(1) If GMDD(U|Z) = 0, then  $n\text{GMDD}_n(U|Z) \xrightarrow{d} \sum_{k=1}^{\infty} \lambda_k G_k^2$ , (5)

where  $\{G_k\}_{k=1}^{\infty}$  is a sequence of iid standard Gaussian random variables, and  $\{\lambda_k\}_{k=1}^{\infty}$ ,  $\lambda_k \ge 0$ , is a sequence of non-increasing coefficients that depend on the distribution of (U, Z) and the kernel  $K(\cdot)$ .

(2) If GMDD(U|Z) > 0, then

$$\sqrt{n}(\mathrm{GMDD}_n(U|Z) - \mathrm{GMDD}(U|Z)) \xrightarrow{d} \mathcal{N}(0, 4\mathrm{Var}\{J(D)\}),$$

where 
$$J(D) := \left\{ \mathbb{E}[(U^{\dagger} - \mathbb{E}U)K(Z - Z^{\dagger})|Z] - \mathbb{E}[(U^{\dagger} - \mathbb{E}U)K(Z - Z^{\dagger})] \right\} (U - \mathbb{E}U), and D = (U, Z).$$

The key observation from Proposition 2.1 is that the limiting behavior of the GMDD-based test statistic is non-pivotal under mean independence. It depends heavily on the underlying data-generating process (DGP) and the integrating measure  $\nu(\cdot)$ . This may hinder the use of GMDD for practitioners because the implementation usually requires bootstrapped critical values. This is precisely the problem rectified by the proposed test in Section 3 while preserving the omnibus property. Although the existing literature is well aware of this problem, e.g., Bierens (1982), Domínguez and Lobato (2004) and Escanciano (2006b), improvements largely remain focused on bootstrap calibration methods, e.g., Domínguez and Lobato (2015), instead of pivotalizing ICM tests.

Another implication of Proposition 2.1 is that  $\text{GMDD}_n(U|Z)$  is first-order degenerate under mean independence, i.e.  $\mathbb{E}[K(Z - Z^{\dagger})(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)|U, Z] = 0$  a.s., which further manifests as J(D) =0 a.s., leading to the breakdown of the central limit theorem. The first-order degeneracy problem is at the heart of the unavailability of pivotal ICM tests, see, e.g., Shao and Zhang (2014, Theorem 4). When mean independence is violated, however,  $\text{GMDD}_n(U|Z)$  is first-order non-degenerate after centering. This suggests a pivotal ICM-based test is achievable once first-order degeneracy under mean independence is appropriately dealt with. In the next section, we further exploit the structure of GMDD and provide a novel perspective for GMDD-based (and thus ICM-based) pivotal tests.

### 3 A new characterization of mean independence

Consider the following hypothesis testing problem of mean independence:

$$\mathbb{H}_{o}: \mathbb{E}[U|Z] = \mathbb{E}[U] \ a.s.;$$

$$\mathbb{H}_{a}: \mathbb{E}[U|Z] \neq \mathbb{E}[U] \ a.s.$$
(6)

The above hypotheses of interest, in view of the omnibus property (3), can be restated as testing GMDD(U|Z) = 0. By the Law of Iterated Expectations (LIE), we have

$$GMDD(U|Z) = -\mathbb{E}\left\{K(Z - Z^{\dagger})(U^{\dagger} - \mathbb{E}U)\mathbb{E}[(U - \mathbb{E}U)|Z, Z^{\dagger}, U^{\dagger}]\right\}$$
  
$$= -\mathbb{E}\left\{K(Z - Z^{\dagger})(\mathbb{E}[U|Z] - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)\right\}.$$
(7)

Under  $\mathbb{H}_o$ ,  $\mathbb{E}[U|Z]$  is degenerate, i.e.,  $\mathbb{E}[U|Z] = \mathbb{E}U$  a.s., which accounts for the first-order degeneracy in Proposition 2.1. In this regard, we propose to replace U with a variable  $V \in \mathbb{R}^{p_v}$  constructed such that  $\mathbb{E}[V|Z]$  is non-degenerate under both the null and alternative hypotheses while preserving the omnibus property. The two crucial properties, namely, the *omnibus* and *first-order non-degeneracy* properties guarantee that the proposed tests are consistent and pivotal. To this end, this paper bases the proposed testing procedure on the quantity

$$\delta_V := \mathbb{E}[K(Z - Z^{\dagger})(V - \mathbb{E}V)(U^{\dagger} - \mathbb{E}U)], \tag{8}$$

where the subscript " $_V$ " is used to reflect the user-dependent choice of V. In (8), we center V around its mean value to align with the expression of GMDD. However, this step can often be omitted with minor adjustments to the theory.

#### 3.1 The Omnibus Property

The omnibus property requires that with a suitable choice of V,  $\delta_V = 0$  if and only if  $\mathbb{H}_o$  holds. The *if part* holds under  $\mathbb{H}_o$  thanks to the degeneracy of  $\mathbb{E}[U|Z]$ . In fact, by the LIE,

$$\delta_{V} = \mathbb{E}\left\{K(Z - Z^{\dagger})(V^{\dagger} - \mathbb{E}V)\mathbb{E}[(U - \mathbb{E}U)|Z, Z^{\dagger}, V^{\dagger}]\right\}$$
  
=  $\mathbb{E}\left\{K(Z - Z^{\dagger})(V^{\dagger} - \mathbb{E}V)(\mathbb{E}[U|Z] - \mathbb{E}U)\right\}.$  (9)

Therefore,  $\mathbb{H}_o$  implies  $\delta_V = 0$  by construction irrespective of the formulation of V. The only if part, which is crucial for the omnibus property of  $\delta_V$ , however, does not hold by construction. We illustrate this by the manipulation of  $\delta_V$  via the LIE. Denote

$$m_{\widetilde{V}}(Z) := \mathbb{E}[K(Z - Z^{\dagger})(V^{\dagger} - \mathbb{E}V)|Z],$$
(10)

then in view of (9), we have

$$\delta_{V} = \mathbb{E} \left\{ \mathbb{E}[K(Z - Z^{\dagger})(V^{\dagger} - \mathbb{E}V)|Z](\mathbb{E}[U|Z] - \mathbb{E}U) \right\}$$
  
=  $\mathbb{E} \left\{ m_{\widetilde{V}}(Z)(\mathbb{E}[U|Z] - \mathbb{E}U) \right\}.$  (11)

Therefore, (11) implies that the only if part fails if  $m_{\tilde{V}}(Z)$  and  $\mathbb{E}[U|Z] - \mathbb{E}U$  are orthogonal to each other under  $\mathbb{H}_a$ .

In view of the preceding, the following condition is imposed to ensure the omnibus property of the

proposed test.

**Condition 3.1** (Omnibus Property). If  $\mathbb{H}_a$  holds, i.e.,  $\mathbb{E}[U|Z] \neq \mathbb{E}U$  a.s., then V is such that

$$\mathbb{E}\{m_{\widetilde{V}}(Z)(\mathbb{E}[U|Z] - \mathbb{E}U)\} \neq 0.$$

Although Condition 3.1 ensures the omnibus property, it imposes a strong restriction on V under  $\mathbb{H}_a$ , which is a high-level condition that does not provide adequate guidance to a practitioner in the specification of V since the direction of  $\mathbb{E}[U|Z]$  under  $\mathbb{H}_a$  is usually unknown. Nevertheless, this condition serves as a guide in the choice of V.

### **3.2** A proposal of V

Since  $\mathbb{E}[U|Z] - \mathbb{E}U \neq 0$  a.s. under  $\mathbb{H}_a$ , and  $K(Z - Z^{\dagger}) \neq 0$  a.s., Condition 3.1 thus implies that  $\mathbb{E}[V^{\dagger}|Z^{\dagger}]$  (or equivalently  $\mathbb{E}[V|Z]$ ) should be non-degenerate under  $\mathbb{H}_a$ . The non-degeneracy of  $\mathbb{E}[V|Z]$  under the  $\mathbb{H}_o$  ensures a pivotal test under the  $\mathbb{H}_o$ . This is stated in the following condition.

Condition 3.2 (First-order non-degeneracy). Under  $\mathbb{H}_o$ ,  $\mathbb{E}[V|Z] \neq \mathbb{E}V$  a.s.

Since V is user-specified, Condition 3.2 can be easily satisfied by letting some components of V be measurable and non-generate functions of Z. Note that the first-order non-degeneracy of  $\mathbb{E}[V|Z]$  should not be understood element-wise, but jointly, in that some *but not all* elements of  $\mathbb{E}[V|Z]$  can be constant almost surely. Condition 3.1 and 3.2, respectively, guarantee the omnibus and first order non-degeneracy properties of  $\delta_V$  under  $\mathbb{H}_o$ . The following fundamental result provides a formulation of V that satisfies Conditions 3.1 and 3.2.

**Lemma 3.1.** For any arbitrary measurable and non-degenerate function h(Z), i.e.,  $h(Z) \neq \mathbb{E}[h(Z)]$  a.s.,  $V = [h(Z), U - h(Z)]^{\top}$  satisfies Conditions 3.1 and 3.2.

*Proof.* Let  $\widetilde{h}(Z) := h(Z) - \mathbb{E}[h(Z)]$ , then

$$\delta_V = \left[ \mathbb{E}[K(Z - Z^{\dagger})\widetilde{h}(Z)(U^{\dagger} - \mathbb{E}U)], -\text{GMDD}(U|Z) - \mathbb{E}[K(Z - Z^{\dagger})\widetilde{h}(Z)(U^{\dagger} - \mathbb{E}U)] \right]^{\top} := [\delta_V^{(1)}, \delta_V^{(2)}]^{\top}.$$

Recall GMDD(U|Z) > 0 under  $\mathbb{H}_a$ , hence  $\delta_V^{(1)} + \delta_V^{(2)} < 0$  under  $\mathbb{H}_a$ . This implies at least one element in  $\delta_V$  is strictly negative (hence strictly different from zero), and thus Condition 3.1 is satisfied. Note that h(Z) is non-degenerate, and that under  $\mathbb{H}_o$ ,  $\mathbb{E}[V|Z] - \mathbb{E}V = [\tilde{h}(Z), \mathbb{E}[U|Z] - \mathbb{E}U - \tilde{h}(Z)]^\top = \tilde{h}(Z)[1, -1]^\top \neq 0$  a.s. It follows that Condition 3.2 holds.

Lemma 3.1 shows that symmetrizing any non-degenerate measurable function of Z about U yields a V that guarantees the omnibus and first-order non-degeneracy properties.

The requirement on h(Z) in Lemma 3.1 can hardly be termed a "condition" as it only requires measurability and non-degeneracy. Therefore, the proposed tests are *omnibus* as long as the choice of Vis suitable, i.e., it obeys Condition 3.1. Moreover, it leads to a first-order non-degenerate U/V-statistics when V obeys Condition 3.2 as well. The proof of Lemma 3.1 provides an insight into the inclusion of U linearly in the construction of V. This brings in the term GMDD(U|Z) in  $\delta_V$  that is strictly positive under  $\mathbb{H}_a$  and drives power under the alternative whenever the "worst-case-scenario" arises when Condition 3.1 is violated with a simple choice such as V = h(Z) under  $\mathbb{H}_a$ . The proposed tests thus draw their consistency from the ICM omnibus property (3).

Since h(Z) can be chosen arbitrarily, the practitioner does not bear the burden of "carefully" selecting functions such as polynomials that provide power by approximating  $\mathbb{E}[U|Z]$  under  $\mathbb{H}_a$ , as required in non-parametric tests specification tests, e.g., Wooldridge (1992), Yatchew (1992), and Zheng (1996). In addition, the user-specified h(Z) provides extra flexibility as the practitioner can use it to augment the power of the test in given directions, unlike GMDD-based bootstrap tests. As demonstrated in Section 4.3, Section 6, and Section S.5.3 of the supplement, properly choosing h(Z) can result in a more powerful test than existing bootstrap-based ICM tests.

**Remark 3.1.** This paper focuses on the fixed-dimensional case. In the high-dimensional setting  $p_z \to \infty$ , Zhang et al. (2018, Remark 2.2) demonstrates that (G)MDD criteria only capture linear dependence when  $p_z$  is large. Our  $\chi^2$ -test derives its consistency property and part of its power from the GMDD so it cannot be expected to perform better in high dimensions.

Furthermore, there are limited efforts in the existing literature dedicated to studying the independence testing problem between two high-dimensional vectors with dimensions p and q, using distance covariancebased test statistics proposed by Székely et al. (2007). In particular, Zhu et al. (2020) shows that if  $\min(p,q) \gg n$ , the distance-based test statistics can only capture the component-wise cross-variance, a phenomenon further supported by Chakraborty and Zhang (2021). Complementing these findings, Gao et al. (2021) shows that if  $p = q = o(\sqrt{n})$ , the re-scaled sample distance correlation can still detect nonlinear dependence. Recently, Zhang et al. (2024) gives a more detailed discussion on how the order of p, q and n can jointly impact the power. Consequently, extending our testing procedure to high dimensions requires a separate paper and is deferred to future research.

### **3.3** Extension to Testing the Nullity of $\mathbb{E}[U|Z]$

In some applications such as specification testing, one may be interested in the nullity of  $\mathbb{E}[U|Z]$ directly, i.e.

$$\mathbb{H}_o^* : \mathbb{E}[U|Z] = 0 \ a.s.; \quad \mathbb{H}_a^* : \mathbb{E}[U|Z] \neq 0.$$

$$\tag{12}$$

This is an augmented version of (6) which further imposes  $\mathbb{E}[U] = 0$ , i.e., a joint hypothesis of conditional mean independence and nullity of the unconditional mean. To this end, we follow Su and Zheng (2017) to augment  $\delta_V$  with an additional quantity that accounts for  $\mathbb{E}[U] = 0$  under  $\mathbb{H}_o^*$ . In particular, one may consider

$$\delta_V^* = \delta_V - \mathbb{E}[K(Z - Z^{\dagger})] \mathbb{E}V \mathbb{E}U.$$

The following result shows that the choice of V in Lemma 3.1 is still valid under such an extension.

**Lemma 3.2.** For V given in Lemma 3.1,  $\delta_V^* = 0$  if and only if  $\mathbb{E}[U|Z] = 0$  a.s.

To save space, we focus on  $\delta_V$  in what follows, and refer the interested reader to Section S.2 of the supplement for the theoretical properties of the  $\chi^2$ -test based on  $\delta_V^*$ .

### 4 Test Statistic and Theoretical Properties

In this section, we construct the test statistic based on  $\delta_V$ . Given empirical observations, in the same spirit of (4), a natural estimator for  $\delta_V$  is given by its sample analogue, i.e.

$$\widehat{\delta}_{V} = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} K(Z_{i} - Z_{j})(U_{i} - \mathbb{E}_{n}[U])(V_{j} - \mathbb{E}_{n}[V]).$$
(13)

In Section 4.1, we analyze the asymptotic behavior of  $\hat{\delta}_V$  under the null hypothesis, as well as under local and fixed alternatives. In Section 4.2, we construct the pivotal  $\chi^2$ -test statistic and discuss its implementation. Section 4.3 uses Bahadur slopes to compare the power of the  $\chi^2$ -test and bootstrapbased GMDD tests.

### 4.1 Asymptotic Distribution

In this section, we analyze the asymptotic behavior of  $\hat{\delta}_V$  under  $\mathbb{H}_o$ , a sequence of Pitman local alternatives

$$\mathbb{H}'_{an}: \mathbb{E}[U|Z] - \mathbb{E}[U] = n^{-1/2}a(Z),$$

and a fixed alternative

$$\mathbb{H}'_a: \mathbb{E}[U|Z] - \mathbb{E}[U] = a(Z),$$

where a(Z) is a non-degenerate measurable function of Z satisfying  $\mathbb{E}[a(Z)] = 0$ . Define D := (U, V, Z),  $m_{\widetilde{U}}(Z) := \mathbb{E}[K(Z - Z^{\dagger})(U^{\dagger} - \mathbb{E}U)|Z],$ 

$$\phi(D) := [m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)](V - \mathbb{E}V) + [m_{\widetilde{V}}(Z) - \mathbb{E}m_{\widetilde{V}}(Z)](U - \mathbb{E}U),$$
(14)

and  $\Omega_V = \operatorname{Var} \{ \phi(D) \}.$ 

Under  $\mathbb{H}_o$ , we have that  $m_{\widetilde{U}}(Z) = 0$  a.s. by the LIE, and hence  $\phi(D)$  reduces to  $\phi(D) = [m_{\widetilde{V}}(Z) - \mathbb{E}m_{\widetilde{V}}(Z)](U - \mathbb{E}U)$ . This implies that  $\Omega_V$  may have different expressions under the null and alternative hypotheses. Here, we distinguish  $\Omega_{V_o}$  and  $\Omega_{V_a}$ , corresponding to specific expressions of  $\Omega_V$  under  $\mathbb{H}_o$ 

and  $\mathbb{H}'_a$ , respectively; they are generally referred to as  $\Omega_V$  whenever the distinction is not needed. For completeness, we impose the following sampling and dominance conditions.

Assumption 4.1.  $\{D_i\}_{i=1}^n$  are independently and identically distributed (iid).

Assumption 4.2.  $\mathbb{E}[||K(Z-Z^{\dagger})VU^{\dagger}||^2] < \infty.$ 

We assume that observations are *iid* in Assumption 4.1 in order to simplify the theoretical analyses. Our results should be extensible to weak temporal dependence, panel data, and clustered data settings, but this lies beyond the scope of the current paper. Assumption 4.2 is standard, e.g., Serfling (2009, Sect. 5.5.1 Theorem A); it is needed to establish the asymptotic normality of  $\sqrt{n}(\hat{\delta}_V - \delta_V)$ .

**Theorem 4.1.** Suppose Assumption 4.1, Assumption 4.2, Condition 3.1, and Condition 3.2 hold, then

- (i) under  $\mathbb{H}_o, \sqrt{n}\widehat{\delta}_V \xrightarrow{d} \mathcal{N}(0, \Omega_{V_o});$
- (ii) under  $\mathbb{H}'_{an}$ ,  $\sqrt{n}\widehat{\delta}_V \xrightarrow{d} \mathcal{N}(a_o, \Omega_{V_o})$ ; and
- (iii) under  $\mathbb{H}'_a$ ,  $\sqrt{n}(\widehat{\delta}_V \delta_V) \xrightarrow{d} \mathcal{N}(0, \Omega_{V_a});$

where  $a_o := \mathbb{E}[(V - \mathbb{E}V)a(Z^{\dagger})K(Z - Z^{\dagger})].$ 

We note that the covariance matrices in the above asymptotic normal distributions can be singular, which we further elaborate on in Section 4.2 below.

#### 4.2 Test Statistic

Theorem 4.1 justifies the asymptotic normality of  $\hat{\delta}_V$ , even under  $\mathbb{H}_o$ , which naturally motivates the Wald test statistic:

$$\widetilde{T}_{V,n} = n \widehat{\delta}_V^\top \widetilde{\Omega}_{V,n}^{-1} \widehat{\delta}_V, \tag{15}$$

where  $\widetilde{\Omega}_{V,n}$  is a consistent estimator of  $\Omega_V$  under both  $\mathbb{H}_o$  and  $\mathbb{H}_a$ . This testing procedure is valid when  $\Omega_V$  is positive definite, which, however, may not be true for our test. For example, the formulation

 $V = [h(Z), U - h(Z)]^{\top}$  in Lemma 3.1 under  $\mathbb{H}_o$  yields

$$\phi(D) = [m_{\widetilde{h}}(Z) - \mathbb{E}m_{\widetilde{h}}Z)](U - \mathbb{E}U) \times [1, -1]^{\top}, \quad \text{with} \quad m_{\widetilde{h}}(Z) := \mathbb{E}\left\{K(Z - Z^{\dagger})[h(Z^{\dagger}) - \mathbb{E}h(Z^{\dagger})]|Z\right\},$$

which is of column rank one. This suggests that  $\Omega_V$  can be singular. Indeed,

$$\Omega_V = \mathbb{E}\left\{ [m_{\tilde{h}}(Z) - \mathbb{E}m_{\tilde{h}}(Z)](U - \mathbb{E}U) \right\}^2 \times \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

Although it is tempting to replace the inverse matrix  $\tilde{\Omega}_{V,n}^{-1}$  in (15) with a generalized inverse matrix  $\tilde{\Omega}_{V,n}^{-}$ , e.g., the Moore-Penrose inverse, the resulting Wald statistic may still not have an asymptotic  $\chi^2$  distribution unless the rank condition,

$$\mathbb{P}\big(\mathrm{rank}(\widehat{\Omega}_{n,V}) = \mathrm{rank}(\Omega_V)\big) \to 1 \quad \text{as } n \to \infty,$$
(16)

is satisfied, see Andrews (1987). To deal with this problem, we adopt the thresholding technique in Lütkepohl and Burda (1997) which ensures the rank condition (16) is satisfied, see also Duchesne and France (2015) and Dufour and Valéry (2016). Let

$$\widetilde{\Omega}_{V,n} = \frac{1}{n-1} \sum_{i=1}^{n} [\widehat{\phi}(D_i) - 2\widehat{\delta}_V] [\widehat{\phi}(D_i) - 2\widehat{\delta}_V]^{\top},$$
(17)

be a consistent estimator of  $\Omega_V$  (Sen, 1960), where

$$\widehat{\phi}(D_i) := [\widehat{m}_{\widetilde{V}}(Z_i) - \mathbb{E}_n \widehat{m}_{\widetilde{V}}(Z)](U_i - \mathbb{E}_n U) + [\widehat{m}_{\widetilde{U}}(Z_i) - \mathbb{E}_n \widehat{m}_{\widetilde{U}}(Z)](V_i - \mathbb{E}_n V_i),$$

and

$$\widehat{m}_{\widetilde{V}}(Z_i) = \frac{1}{n-1} \sum_{j=1, j \neq i} K(Z_i - Z_j)(V_j - \mathbb{E}_n V), \quad \widehat{m}_{\widetilde{U}}(Z_i) = \frac{1}{n-1} \sum_{j=1, j \neq i} K(Z_i - Z_j)(U_j - \mathbb{E}_n U).$$

By the singular value decomposition,

$$\widetilde{\Omega}_{V,n} = \widetilde{\Gamma}_n \widetilde{\Lambda}_n \widetilde{\Gamma}_n^{\top}, \tag{18}$$

where  $\widetilde{\Lambda}_n = \operatorname{diag}(\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_{p_v})$  is the diagonal matrix comprising the eigenvalues  $\widetilde{\lambda}_1 \geq \dots \geq \widetilde{\lambda}_{p_v} \geq 0$  of  $\widetilde{\Omega}_{V,n}$ , and the columns of  $\widetilde{\Gamma}_n$  are the corresponding eigenvectors. For  $c_n = Cn^{-1/2+\iota}$  where  $\iota \in (0, 1/2)$  is a small positive number and  $C \in (0, \infty)$  is a constant (Dufour & Valéry, 2016), we define the regularized estimator of  $\Omega_V$  by

$$\widehat{\Omega}_{V,n} := \widetilde{\Gamma}_n \widehat{\Lambda}_{n,c_n} \widetilde{\Gamma}_n^{\top}, \text{ where } \widehat{\Lambda}_{n,c_n} = \operatorname{diag}(\widetilde{\lambda}_1 \mathbf{1}(\widetilde{\lambda}_1 > c_n), \cdots, \widetilde{\lambda}_{p_v} \mathbf{1}(\widetilde{\lambda}_{p_v} > c_n))$$
(19)

and its Moore-Penrose inverse by

$$\widehat{\Omega}_{V,n}^{-} := \widetilde{\Gamma}_n \widehat{\Lambda}_{n,c_n}^{-} \widetilde{\Gamma}_n^{\top} \text{ where } \widehat{\Lambda}_{n,c_n}^{-} = \text{diag}(\widetilde{\lambda}_1^{-1}, \cdots, \widetilde{\lambda}_{p(c_n)}^{-1}, \mathbf{0}_{p_v - p(c_n)}^{\top})$$

and  $p(c_n) = \sum_{l=1}^{p_v} \mathbb{1}\{\widetilde{\lambda}_l > c_n\}.$ 

Finally, we define the regularized Wald test statistic:

$$T_{V,n} := n \widehat{\delta}_V^\top \widehat{\Omega}_{V,n}^- \widehat{\delta}_V.$$
<sup>(20)</sup>

In practice,  $\mathbb{H}_o$  is rejected when  $T_{V,n} > \chi^2_{\operatorname{rank}(\Omega_{V_o}),1-\alpha}$ , the  $1-\alpha$  quantile of  $\chi^2_{\operatorname{rank}(\Omega_{V_o})}$ , at a pre-specified significance level  $\alpha \in (0,1)$ . We remark that  $\Omega_{V_o}$  and  $\Omega_{V_a}$  can be different, for example, for V in Lemma 3.1,  $\operatorname{rank}(\Omega_{V_o}) = 1$  while  $\operatorname{rank}(\Omega_{V_a}) = 2$  if  $a(Z) \neq c \cdot h(Z)$  for any  $c \in \mathbb{R}$ .

**Remark 4.1.** Following Lütkepohl and Burda (1997) and Dufour and Valéry (2016), a consistent choice of the threshold  $c_n$  that is used in this paper is  $c_n = \tilde{\lambda}_1 n^{-1/3}$  where  $\tilde{\lambda}_1$  is the leading eigenvalue of  $\tilde{\Omega}_{V,n}$ . For the robustness of the  $\chi^2$ -test to variations of the form  $c_n = \tilde{\lambda}_1 n^{-\iota}$ ,  $\iota \in (0, 1/2)$  and other suitable selection criteria commonly used in the literature on truncated singular value decomposition, see Section S.5.4 in the supplement. **Remark 4.2.** In general, rank( $\Omega_{V_o}$ ) is the number of free elements in  $\mathbb{E}[V|Z]$  under  $\mathbb{H}_o$  that cannot be expressed almost surely as a linear combination of the other elements. For example, when V takes the bivariate form in Lemma 3.1, rank( $\Omega_{V_o}$ ) = 1. Under  $\mathbb{H}_o$ , GMDD<sub>n</sub>(U|Z) =  $O_p(n^{-1})$  from (5) in Proposition 2.1, thus it can be shown that  $\sqrt{n}\delta_V = \sqrt{n}\delta_V^{(1)}[1, -1]^\top + O_p(n^{-1/2})$ . In this particular case, the test statistic has the form

$$T_{V,n} = n\widehat{\delta}_V^{\top}\widehat{\Omega}_{V,n}^{-}\widehat{\delta}_V = \left(\frac{\widehat{\delta}_V^{(1)}}{\sqrt{\operatorname{Var}(\widehat{\delta}_V^{(1)})}}\right)^2 + o_p(1) \xrightarrow{d} \chi_1^2, \quad as \quad n \to \infty.$$

This implies  $\sqrt{T_{V,n}}$  converges in distribution to the half standard normal under  $\mathbb{H}_o$  and shares the interpretability without a formal hypothesis test of a two-sided t-test.

The next theorem justifies the use of (20) under the null hypothesis, local alternatives, and fixed alternatives.

**Theorem 4.2.** If  $\mathbb{E} |\psi(D_i, D_j)|^{4+\varepsilon} < \infty$  for some  $\varepsilon > 0$ , and let  $c_n = Cn^{-1/2+\iota}$  for some constants  $\iota \in (0, 1/2)$  and  $C \in (0, \infty)$  independent of n, then

(i) under  $\mathbb{H}_o, \ \widehat{\Omega}_{V,n}^- \xrightarrow{p} \Omega_{V_o}^-$ , and

$$T_{V,n} \xrightarrow{d} \chi^2_{\operatorname{rank}(\Omega_{V_o})};$$

(ii) under  $\mathbb{H}'_{an}$ ,  $\widehat{\Omega}^{-}_{V,n} \xrightarrow{p} \Omega^{-}_{V_{o}}$ , the asymptotic local power is given by

$$\lim_{n \to \infty} \mathbb{P}(T_{V,n} > \chi^2_{\operatorname{rank}(\Omega_{V_o}), 1-\alpha}) = \mathbb{P}\left(\chi^2_{\operatorname{rank}(\Omega_{V_o})}(\theta) > \chi^2_{\operatorname{rank}(\Omega_{V_o}), 1-\alpha}\right),$$

where  $\theta := a_o^\top \Omega_{V_o}^- a_o$ ,  $a_o$  is defined in Theorem 4.1, and  $\chi^2_{\operatorname{rank}(\Omega_{V_o})}(\theta)$  is a non-central  $\chi^2$  random variable; and

(iii) under  $\mathbb{H}'_a$ ,  $\widehat{\Omega}^-_{V,n} \xrightarrow{p} \Omega^-_{V_a}$ , and if  $\delta_V \notin \mathcal{M}_0$ , where  $\mathcal{M}_0$  is the eigenspace associated with the null eigenvalue of  $\Omega_{V_a}$ ,

$$\lim_{n \to \infty} \mathbb{P}(T_{V,n} > \chi^2_{\operatorname{rank}(\Omega_{V_o}), 1-\alpha}) = 1.$$

**Remark 4.3.** For V defined in Lemma 3.1,  $\delta_V \notin \mathcal{M}_0$  always holds and hence the test given Theorem 4.2 (iii) is consistent. The proof is provided in the supplementary material.

### 4.3 Power Comparison with the GMDD test

In this section, we examine the efficiency of the proposed test statistic compared with the bootstrapbased GMDD test by adopting the approach of Bahadur (1960). Under a fixed alternative, both tests demonstrate consistency as n tends to infinity. The Bahadur slope in Bahadur (1960) allows us to further compare the rate of convergence of p-values to zero as n increases.

Let  $S_G(t) := \mathbb{P}(\sum_{k=1}^{\infty} \lambda_k G_k^2 > t)$  and  $S_T(t) := \mathbb{P}(\chi^2_{\operatorname{rank}(\Omega_{V_o})} > t)$  be the survival functions of the asymptotic null distributions of the GMDD test statistic  $n \operatorname{GMDD}_n(U|Z)$ , and the pivotal test statistic,  $T_{V,n}$ , respectively. Their Bahadur slopes are respectively given by

$$c_G = \lim_{n \to \infty} -\frac{2}{n} \log S_G(n \text{GMDD}_n(U|Z)), \quad c_T = \lim_{n \to \infty} -\frac{2}{n} \log S_G(T_{V,n})$$

**Theorem 4.3.** Suppose  $\widehat{\Omega}_{V,n}^- \xrightarrow{p} \Omega_{V_a}^-$ , and the conditions of Theorem 4.2 hold, then under  $\mathbb{H}'_a : \mathbb{E}[U|Z] - \mathbb{E}[U] = a(Z)$ , where a(Z) is a non-degenerate function of Z, the (approximate) Bahadur slopes of the GMDD test statistic  $n\text{GMDD}_n(U|Z)$  and the pivotal test statistic  $T_{V,n}$  are respectively given by

$$c_G = \frac{-\mathbb{E}[a(Z)a(Z^{\dagger})K(Z-Z^{\dagger})]}{\lambda_1} \quad and \ c_T = a_o^{\top}\Omega_{V_a}^{-}a_o^{\top}$$

where  $\lambda_1$  is the leading eigenvalue associated with the limiting null distribution in (5), and  $a_o = \mathbb{E}[(V - \mathbb{E}V)a(Z^{\dagger})K(Z - Z^{\dagger})].$ 

The approximate Bahadur slopes presented in Theorem 4.3 are primarily of theoretical interest. Conducting a comprehensive comparison of these slopes is challenging as they depend on data-dependent quantities such as  $\lambda_1$  and a(Z) and user-specified variables like V and the kernel  $K(\cdot)$ .

To make these results concrete, we consider the simple design

$$U = \exp(-Z^2/3) - \sqrt{3/5} + \mathcal{E}$$
, with  $Z \sim \mathcal{N}(0, 1)$  and  $\mathcal{E} \sim \mathcal{U}[-\sqrt{3}, \sqrt{3}]$ 

where  $\mathcal{E}$  is independent of Z, hence  $\mathbb{E}[U|Z] := a(Z) = \exp(-Z^2/3) - \sqrt{3/5}$ , and  $\mathbb{E}U = 0.^1$  Using the Gaussian kernel  $K(Z - Z^{\dagger}) = \exp(-0.5(Z - Z^{\dagger})^2)$  for both tests, Table 4.1 shows the Bahadur slopes of the GMDD test alongside the  $\chi^2$ -test with

(1) 
$$V_1 = [h_1(Z), U - h_1(Z)]^\top, h_1(Z) = \exp(Z) - \exp(1/2)$$
 which is agnostic of  $a(Z)$ ;

- (2)  $V_{1a} = [h_1(Z), U h_1(Z), Z]^\top;$
- (3)  $V_2 = [h_2(Z), U h_2(Z)]^{\top}, h_2(Z) = a(Z)$  which results in a singular covariance matrix under  $\mathbb{H}_a$ ;
- (4)  $V_3 = [h_3(Z), \ U h_3(Z)]^\top, \ h_3(Z) = \sqrt{3} \exp(-Z^2/2) \sqrt{3/2}$  which satisfies  $\mathbb{E}[K(Z Z^{\dagger})h(Z^{\dagger})|Z] = \exp(-Z^2/3) \sqrt{3/5} := a(Z);$  and
- (5)  $V_{3a} = [h_3(Z), U h_3(Z), Z]^\top$ .

In scenarios (3) - (5), we use prior knowledge of the alternative. In (3), it can be shown that  $a_o = -[\text{GMDD}(U|Z), 0]^{\top}$ , and

$$\Omega_{V_a} = A \times \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

where  $A = \text{Var} \{\phi(D)\}$  and  $\phi(D) = (U - \mathbb{E}U)\mathbb{E}[a(Z^{\dagger})K(Z - Z^{\dagger})|Z]$ . Clearly,  $\mathbb{E}[\phi(D)] = -\text{GMDD}(U|Z)$ , therefore  $a_o^{\top}\Omega_{V_a}^{-}a_o = \text{GMDD}^2(U|Z)/[4\text{Var}(\phi(D))]$ . This is in fact a worst-case scenario under  $\mathbb{H}_a$  for the  $\chi^2$ -test. To fully make use of the information of a(Z), the choice of h(Z) in scenario (4) maximizes the linear dependence in Condition 3.1 with respect to the first element of  $\delta_V$  while the second term is not degenerate:  $\delta_V = \mathbb{E}[a^2(Z), -\text{GMDD}(U|Z) - a^2(Z)]^{\top}$ . Therefore, power should be augmented. Scenarios (2) and (5) are Vs of scenarios (1) and (4) augmented with Z.

Table 4.1: Bahadur Slopes

	GMDD			$\chi^2$		
		$V_1$	$V_{1a}$	$V_2$	$V_3$	$V_{3a}$
Bahadur Slope	0.0109	0.0214	0.0242	0.0056	0.0246	0.0246

<sup>1</sup>See Appendix S.6 for details on the computation of the Bahadur slopes.

Table 4.1 shows that the GMDD is an intermediate case between the agnostic choice with  $h(Z) = \exp(Z) - \exp(1/2)$  (scenario (1)) and the worst case with h(Z) = a(Z) (scenario (3)). In the case where the linear dependence under Condition 3.1 is maximized with respect to either element of  $V = [h(Z), U - h(Z)]^{\top}$  without degeneracy in the other (scenario (4)), the  $\chi^2$ -test Bahadur slope is larger. Moreover, we note that when augmenting V, one observes a slight increase in the Bahadur slope for scenario (2) but none for scenario (5). The latter case is not surprising as Z is orthogonal to the direction under alternative, namely,  $\mathbb{E}[K(Z - Z^{\dagger})h(Z^{\dagger})|Z] = a(Z) = \exp(-Z^2/3) - \sqrt{3/5}$  is orthogonal to Z thus the augmentation with Z does not improve power.

### 5 Specification Testing

This section studies the behavior of the  $\chi^2$ -test (20) when applied to the specification testing problem. Specification tests assess conditional moment restrictions which arise often in empirical work. Examples include treatment effect analyses (e.g., Callaway and Karami, 2022), Euler and Bellman equations (Escanciano, 2018; Hansen & Singleton, 1982), the hybrid New Keynesian Phillips curve (Choi et al., 2021), forecast rationality (Hansen & Hodrick, 1980), conditional equal and predictive ability (Giacomini & White, 2006), see Li et al. (2022) for a discussion.

Consider the following parametric regression model,

$$Y_i = g(X_i; \beta_o) + U_i, \tag{21}$$

where  $Y_i \in \mathbb{R}$  is the response variable,  $X_i \in \mathbb{R}^{p_x}$  is the regressor,  $U_i$  is the model error satisfying  $\mathbb{E}[U|Z] = 0$ , and  $Z_i \in \mathbb{R}^{p_z}$  is a vector of instruments which may or may not coincide with  $X_i$ , thus allowing for endogenous  $X_i$ . Here, the regression function  $g(x; \beta_o)$  is known, and parameterized by  $\beta_o \in \mathcal{B}$  where  $\mathcal{B}$  is a compact parameter space in  $\mathbb{R}^k$ .

#### 5.1 The test statistic

The specification testing problem is of the form,

$$\mathbb{H}_{o}: \mathbb{P}(\mathbb{E}[Y_{i} - g(X_{i}; \beta_{o}) | Z_{i}] = 0) = 1, \quad \text{for some } \beta_{o} \in \mathcal{B} \text{ and} 
\mathbb{H}_{a}: \mathbb{P}(\mathbb{E}[Y_{i} - g(X_{i}; \beta) | Z_{i}] = 0) < 1, \quad \text{for all } \beta \in \mathcal{B}.$$
(22)

Note (22) is equivalent to testing  $\mathbb{E}[U_i|Z_i] = 0$  a.s. under the null hypothesis. Unlike the mean independence testing problem in Section 3 where all variables are observed, the error term in (21) is unobservable but can be estimated using the residual

$$\widehat{U}_i = Y_i - g(X_i; \widehat{\beta}_n),$$

where  $\widehat{\beta}_n$  is an estimator of  $\beta_o$ . Similarly, the construction of  $V = \mathcal{V}(U_i, Z_i)$ , which satisfies both the omnibus and first-order non-degeneracy properties in Section 3.1, is replaced with  $\widehat{V}_i = \mathcal{V}(\widehat{U}_i, Z_i)$ . We use the normalization  $\mathbb{E}_n \widehat{U} = 0$  which holds by construction with the inclusion of an intercept term for  $\mathbb{E}U$ . Therefore, one may consider

$$\widehat{\delta}_n = \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} K(Z_i - Z_j) \widehat{U}_i \widehat{V}_j,$$

as the test statistic for specification testing. Note that both  $\hat{U}_i$  and  $\hat{V}_i$  may involve estimation effects, which is shown to have a non-negligible effect on asymptotic properties in comparison to (13).

**Remark 5.1.** A choice of test statistic based on the GMDD metric in the ICM literature is given by  $n\text{GMDD}_n(\hat{U}|Z)$ , where a special case using the MDD metric is considered in Su and Zheng (2017). However, as indicated by results of Proposition 2.1 in the current paper and Theorem 3.1 in Su and Zheng (2017), the asymptotic behavior of  $n\text{GMDD}_n(\hat{U}|Z)$  depends on the underlying data-generating process. More importantly, it is not pivotal. Bootstrap methods are required to obtain asymptotically valid p-values for statistical inference.

Given the above remark, we will not investigate the theoretical properties of  $n \text{GMDD}_n(\widehat{U}|Z)$ , for which

proof techniques developed for Section 2 and Su and Zheng (2017) are applicable.

### 5.2 Asymptotic Theory

Following Bierens and Ploberger (1997) and Escanciano (2009), we consider the asymptotic behavior of  $\hat{\delta}_n$  under the following sequence of Pitman local alternatives

$$\mathbb{H}_{an}: Y_i = g(X_i; \beta_0) + n^{-1/2} a(X_i, Z_i) + \mathcal{E}_i, \quad i = 1, \dots, n,$$
(23)

where  $\mathcal{E}_i := Y_i - \mathbb{E}[Y_i|Z_i]$  and  $U_i = \mathcal{E}_i + n^{-1/2}a(X_i, Z_i)$ . As the form of misspecification  $a(X_i, Z_i)$  contains both  $X_i$  and  $Z_i$ , it also allows for misspecification that violates the IV exclusion restriction on excluded instruments in Z. From (23),  $\mathcal{E}_i = U_i$  under  $\mathbb{H}_o$ . The following conditions are imposed.

Condition 5.1.  $\mathbb{E}[U^2 + K^2(Z)] < \infty$ .

**Condition 5.2.** (i).  $g'(x;\beta) := \partial g(x;\beta)/\partial \beta$  exists and is a continuously differentiable function of  $\beta \in \mathcal{B}$ on the support of  $X_i$ ; (ii)  $\mathbb{E}[\sup_{\beta \in \mathcal{B}} ||g'(X_i;\beta)||] < \infty$ .

Condition 5.3.  $\beta_o$  is an interior point of  $\mathcal{B}$  and there exists a consistent estimator  $\hat{\beta}_n$  of  $\beta_o$  that satisfies: (i).

$$\sqrt{n}(\widehat{\beta}_n - \beta_o) = \zeta_a + \frac{1}{\sqrt{n}} \sum_{i=1}^n \varphi_i \mathcal{E}_i + o_p(1),$$

where  $\zeta_a = \mathbb{E}[a(X_i, Z_i)\varphi_i] \in \mathbb{R}^k$ ,  $\varphi_i := \varphi_i(\beta_o) = \varphi(X_i, Z_i; \beta_o)$  with  $\mathbb{E}[\mathcal{E}_i\varphi_i] = 0$  and  $\varphi_i(\beta) \in \mathbb{R}^k$  is observable for given  $\beta \in \mathcal{B}$ ;

(ii).  $\Xi_0 := \mathbb{E}[\varphi_i \varphi_i^\top \mathcal{E}_i^2]$  exists and is positive definite.

Condition 5.4.  $\widehat{V}_i = \mathcal{V}(\widehat{U}_i, Z_i) \in \mathbb{R}^{p_v}$ , and satisfies:

*(i)*.

$$\widehat{V}_i = V_i + \xi_i^\top (\widehat{\beta}_n - \beta_o) + o_p(n^{-1/2}),$$

where  $V_i = \mathcal{V}(U_i, Z_i)$  satisfies Condition 3.2,  $\xi_i := \xi_i(\beta_o) = \xi(X_i, Z_i; \beta_o) \in \mathbb{R}^{k \times p_v}$ , and  $\xi_i(\beta) \in \mathbb{R}^{k \times p}$  is observable for given  $\beta \in \mathcal{B}$ ;

(*ii*).  $\mathbb{E} \|\xi_i\|^2 < \infty$ .

The above assumptions are standard in the specification testing literature, cf. Bierens (1982), Escanciano (2009), and Su and Zheng (2017). Condition 5.1 imposes moment conditions on the data and the kernel used, which ensures that the GMDD metric is well defined. Although the moment restriction on U cannot be relaxed, that of  $K(\cdot)$  can be relaxed through the choice of bounded kernels or suitable transformations of Z – see Remark 2.1. Condition 5.2 regulates the smoothness and moment conditions of the nonlinear regression function  $g(x;\beta)$ . Condition 5.3 follows Assumption A3 in Escanciano (2009) and assumes that the estimator  $\hat{\beta}_n$  is consistent and permits a Bahadur linear representation under  $\mathbb{H}_{an}$ . Condition 5.3(ii) requires instrument relevance, e.g.,  $\mathbb{E}[Z^{\top}X]$  is non-singular in the case of the linear IV estimator. The Bahadur linear representation holds for a large class of estimators defined by estimating equations, including commonly used (nonlinear) least squares, maximum likelihood, and GMM estimators. Condition 5.4 is similar to Condition 5.3, and is satisfied when the function  $\mathcal{V}(\cdot, Z)$  is twice continuously differentiable in the neighborhood of  $\beta_o$  by a standard Taylor expansion argument. In particular, if the construction of  $\hat{V}$  does not depend on  $\hat{U}$ , we set  $\xi = 0$ .

We are now ready to establish the asymptotic distribution of  $\sqrt{n}\hat{\delta}_n$  under  $\mathbb{H}_{an}$  (hence  $\mathbb{H}_o$ ). Define  $\psi(D_i, D_j) = K(Z_i - Z_j)(\mathcal{E}_i V_j + \mathcal{E}_j V_i)$ , and  $\psi^{(1)}(D_i) = \mathbb{E}[\psi(D_i, D_j)|D_i]$ . Moreover, define

$$r_{i} := \partial g(X_{i}; \beta_{o}) / \partial \beta_{o} \in \mathbb{R}^{k}, \quad \Xi_{1} = -\mathbb{E}[K(Z_{i} - Z_{j})V_{j}r_{i}^{\top}] \in \mathbb{R}^{p_{v} \times k},$$
  

$$\Xi_{2} = \mathbb{E}[\psi^{(1)}(D_{i})\mathcal{E}_{i}\varphi_{i}^{\top}] \in \mathbb{R}^{p_{v} \times k}, \quad \Xi_{a} = \mathbb{E}[K(Z_{i} - Z_{j})a(X_{i}, Z_{i})\widetilde{V}_{j}] \in \mathbb{R}^{p_{v}}, \text{ and}$$
  

$$\Omega_{\delta} = \operatorname{Var}\{\psi^{(1)}(D_{i})\} + \Xi_{1}\Xi_{0}\Xi_{1}^{\top} + \Xi_{1}\Xi_{2}^{\top} + \Xi_{2}\Xi_{1}^{\top}.$$
(24)

**Theorem 5.1.** Suppose Conditions 5.1-5.4 hold, then, under  $\mathbb{H}_{an}$ ,

$$\sqrt{n}\widehat{\delta}_n \xrightarrow{d} \mathcal{N}(\Xi_a + \Xi_1\zeta_a, \ \Omega_\delta).$$

In particular, under  $\mathbb{H}_o$ ,

$$\sqrt{n}\widehat{\delta}_n \xrightarrow{d} \mathcal{N}(0,\Omega_\delta).$$

Compared with the asymptotic results in Theorem 4.1, the asymptotic variance in the above theorem corrects for the additional effect of estimating  $\beta_o$ , see Condition 5.3 and Condition 5.4. Such estimation effect contributes  $\Xi_1 \zeta_a$  to the local power in addition to the part  $\Xi_a$  that stems from model misspecification. In practice,  $\Omega_{\delta}$  can be estimated by replacing the quantities that appear in (24) with their sample counterparts. Let

$$\widehat{\psi}^{(1)}(D_i) = \frac{1}{(n-1)} \sum_{j=1, j \neq i}^n K(Z_i - Z_j) \left( \widehat{U}_i \widehat{V}_j + \widehat{U}_j \widehat{V}_i \right),$$

and define the corresponding sample estimators:

$$\begin{split} \widetilde{\Omega}_{\delta,n} &= \widetilde{\Omega}_{V,n} + \widetilde{\Xi}_{1,n} \widetilde{\Xi}_{0,n} \widetilde{\Xi}_{1,n}^{\top} + \widetilde{\Xi}_{1,n} \widetilde{\Xi}_{2,n}^{\top} + \widetilde{\Xi}_{2,n} \widetilde{\Xi}_{1,n}^{\top}; \\ \widetilde{\Omega}_{V,n} &= \frac{1}{n} \sum_{i=1}^{n} [\widehat{\psi}^{(1)}(D_{i}) - 2\widehat{\delta}_{n}] [\widehat{\psi}^{(1)}(D_{i}) - 2\widehat{\delta}_{n}]^{\top}; \\ \widetilde{\Xi}_{0,n} &= \frac{1}{n} \sum_{i=1}^{n} \varphi(X_{i}, Z_{i}; \widehat{\beta}_{n}) \varphi(X_{i}, Z_{i}; \widehat{\beta}_{n})^{\top} \widehat{U}_{i}^{2}; \\ \widetilde{\Xi}_{1,n} &= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i}^{n} K(Z_{i} - Z_{j}) [\widehat{U}_{i}\xi(X_{j}, Z_{j}; \widehat{\beta}_{n})^{\top} - \widehat{V}_{j}g'(X_{i}; \widehat{\beta}_{n})^{\top}]; \text{ and} \\ \widetilde{\Xi}_{2,n} &= \frac{1}{n} \sum_{i=1}^{n} \widehat{\psi}^{(1)}(D_{i}) \widehat{U}_{i} \varphi(X_{i}, Z_{i}; \widehat{\beta}_{n})^{\top}. \end{split}$$

The regularized Wald test statistic in the same spirit as (20) can be defined as

$$T_n = n\widehat{\delta}_n^\top \widehat{\Omega}_{\delta,n}^- \widehat{\delta}_n,$$

where  $\widehat{\Omega}_{\delta,n}^{-}$  is the Moore-Penrose inverse of  $\widehat{\Omega}_{\delta,n}$ , which is constructed similarly as in (18) and (19).

We reject  $\mathbb{H}_o$  when  $T_n > \chi^2_{\operatorname{rank}(\Omega_{\delta_o}),1-\alpha}$  where  $\chi^2_{\operatorname{rank}(\Omega_{\delta_o}),1-\alpha}$  is the  $1-\alpha$  quantile of the  $\chi^2_{\operatorname{rank}(\Omega_{\delta_o})}$  and  $\operatorname{rank}(\Omega_{\delta_o})$  is the rank of  $\Omega_{\delta}$  under  $\mathbb{H}_o$ . For practical implementation,  $\operatorname{rank}(\Omega_{\delta_o})$  has to be predetermined, which may be further complicated by the estimation effect compared with the case of  $\Omega_{V_o}$  in the test of mean independence in Section 4.1. Luckily, the following lemma shows that such estimation effect on the rank is negligible for a specification test with the formulation  $\widehat{V}_i = [h(Z_i), \ \widehat{U}_i - h(Z_i)]^{\top}$ .

**Lemma 5.1.** Under the conditions of Theorem 5.1, the formulation  $\widehat{V}_i = [h(Z_i), \ \widehat{U}_i - h(Z_i)]^\top$  satisfies  $\operatorname{rank}(\Omega_{\delta_o}) = \operatorname{rank}(\Omega_{V_o}) = 1$  under  $\mathbb{H}_o$ , where  $h(\cdot)$  is a measurable and non-degenerate function of  $Z_i$ .

Therefore, in practice, one only needs to determine  $\operatorname{rank}(\Omega_{V_o})$ , which depends on the user-specified V. In view of Remark 4.2 and Lemma 5.1, the  $\chi^2$ -test procedures based on  $V = [h(Z), U - h(Z)]^{\top}$  do not require the estimation of  $\operatorname{rank}(\Omega_{V_o})$ .

# 6 Monte Carlo Experiments - Specification Test

This section examines the size and power of the  $\chi^2$  specification test with  $\hat{V} = [h(Z), \hat{U} - h(Z)]$ in comparison to bootstrap-based ICM procedures via simulations.<sup>2</sup> For all implementations of the specification test proposed in this paper, the regularized inverse in (15) is computed using  $c_n = \tilde{\lambda}_1 n^{-1/3}$ where  $\tilde{\lambda}_1$  is the leading eigenvalue of  $\tilde{\Omega}_{V,n}$ .<sup>3</sup> For ease of exposition, we choose the Gaussian kernel  $K(Z - Z^{\dagger}) = \exp(-0.5||Z - Z^{\dagger}||^2)$  for the GMDD measure as other kernels deliver similar results. The following ICM metrics are considered for the bootstrap procedures: Gaussian (Gauss), S&Z (corresponding to the Su and Zheng (2017) test), and the angular distance (Esc6) of Escanciano (2006a). The empirical size and power curves are based on 1000 Monte Carlo replicates. 499 bootstrap samples are used for the bootstrap procedures.<sup>4</sup> Other simulation results on specification and mean independence tests are relegated to Section S.5 of the supplementary material.

#### 6.1 Specifications

We consider the linear model

$$Y = X + U,$$

with and without excluded instruments based on the following DGPs of U:

 $<sup>^{2}</sup>$ See Section S.5 in the supplement for simulation results on the test of mean independence.

<sup>&</sup>lt;sup>3</sup>For the robustness of the performance of the proposed  $\chi^2$ -test to other suitable selection criteria, see Section S.5.4 in the supplement.

 $<sup>^{4}</sup>$ The wild bootstrap with Mammen (1993) two-point distributed auxiliary variables is used to conduct all bootstrap-based ICM tests.

LS1: 
$$U = \frac{\mathcal{E}}{\sqrt{1+Z^2}}$$
;  
LS2:  $U = \frac{\sqrt{2}}{5}\gamma Z^2 + \frac{\mathcal{E}}{\sqrt{1+Z^2}}$ ;  
LS3:  $U = 2.5\frac{Z^2}{\sqrt{n}} + \frac{\mathcal{E}}{\sqrt{1+Z^2}}$ ;  
LS4:  $U = 0.5\gamma \frac{\sin(2Z) + \cos(2Z)}{\sqrt{(1-\exp(-8))/2}} + \frac{\mathcal{E}}{\sqrt{1+Z^2}}$ ; and  
LS5:  $U = \exp(-Z^2/3) - \sqrt{3/5} + \frac{\mathcal{E}}{\sqrt{1+Z^2}}$ 

where  $\mathcal{E}$  and Z are independent  $\mathcal{N}(0,1)$  random variables, and  $\gamma \in [0,1]$  tunes the deviation away from  $\mathbb{H}_o$ . In the above specifications, we set X = Z in DGP LS1 and  $X = (1.5Z + \tilde{\mathcal{E}})/\sqrt{3.25}$  with  $\tilde{\mathcal{E}} \sim \mathcal{N}(0,1)$  and  $\text{Cov}(\tilde{\mathcal{E}}, \mathcal{E}) = 0.5$  in DGPs LS2 through LS5. Thus, X is exogenous under DGP LS1 and endogenous under DGPs LS2 through LS5. LS1 is estimated via Ordinary Least Squares (OLS) while the rest are estimated using the Instrumental Variable (IV) estimator with Z as the excluded instrument. Observe that heteroskedasticity of arbitrary form is imposed in all DGPs.

Different sample sizes  $n \in \{200, 400, 600, 800\}$  help to examine the empirical size of the test in DGPs LS1 and LS2 (with  $\gamma = 0$ ). For the analyses of (local) power in DGPs LS2 through LS5, the sample size is kept at n = 400 while  $\gamma$  is varied in order to study the power of the proposed  $\chi^2$ -test in comparison to the bootstrap-based ICM procedures.

#### 6.2 Empirical Size and Power

Table 6.1 presents the empirical sizes corresponding to DGPs LS1 (under strictly exogenous X) and LS2 (under endogenous X instrumented with Z) at three nominal levels: 10%, 5%, and 1%. One observes comparably good size control of the proposed  $\chi^2$ -test and the wild-bootstrap-based procedures across all the sample sizes considered. This lends evidence to the proposed test's validity under both exogenous Xand endogenous X with valid instrument Z.

To ensure that the good size control of the  $\chi^2$ -test in Table 6.1 is not achieved at the expense of power, we consider its performance under both local and fixed alternatives. DGP LS3 serves to examine

		10	%			50	%			10	70	
n	$\chi^2$	Gauss	S&Z	Esc6	$\chi^2$	Gauss	S&Z	Esc6	$\chi^2$	Gauss	S&Z	Esc6
LS1												
200	0.112	0.071	0.081	0.077	0.068	0.034	0.033	0.035	0.022	0.011	0.006	0.007
400	0.097	0.091	0.096	0.091	0.058	0.041	0.042	0.047	0.011	0.004	0.006	0.008
600	0.111	0.107	0.107	0.101	0.052	0.058	0.050	0.052	0.012	0.010	0.010	0.006
800	0.110	0.091	0.089	0.087	0.047	0.048	0.051	0.050	0.012	0.012	0.013	0.011
LS2												
200	0.111	0.069	0.084	0.077	0.074	0.038	0.033	0.036	0.023	0.011	0.006	0.006
400	0.101	0.090	0.097	0.093	0.058	0.041	0.044	0.043	0.012	0.004	0.007	0.006
600	0.112	0.106	0.105	0.105	0.054	0.057	0.051	0.054	0.013	0.010	0.010	0.007
800	0.108	0.093	0.089	0.090	0.046	0.048	0.050	0.050	0.014	0.012	0.013	0.009

Table 6.1: Empirical Size - DGP LS1 & LS2

power under the local alternative. The results are presented in Table 6.2. Clearly, the local power of the proposed  $\chi^2$ -test alongside the bootstrap-based procedures is non-trivial.

Table 6.2: Local Power – DGP LS3

		10%				50	70		1%			
n	$\chi^2$	Gauss	S&Z	Esc6	$\chi^2$	Gauss	S&Z	Esc6	$\chi^2$	Gauss	S&Z	Esc6
LS2												
200	0.978	0.984	0.981	0.923	0.937	0.962	0.953	0.853	0.757	0.862	0.815	0.625
400	0.988	0.990	0.992	0.946	0.974	0.978	0.974	0.884	0.882	0.904	0.872	0.690
600	0.991	0.992	0.987	0.944	0.976	0.974	0.968	0.898	0.903	0.925	0.904	0.736
800	0.993	0.993	0.992	0.954	0.984	0.990	0.981	0.903	0.928	0.925	0.906	0.742

Figures 1 to 3 present power curves corresponding to DGPs LS2, LS4, and LS5, respectively. From Figures 1 to 3, one observes that all tests demonstrate non-trivial power against the fixed alternative for variations of  $\gamma$  away from zero. Quite interestingly, the  $\chi^2$ -test slightly dominates the bootstrap-based procedures in terms of power in Figure 2 while remaining competitive in Figure 1.



Figure 1: Power Curves - DGP LS2, n = 400.



Figure 2: Power Curves - DGP LS4, n = 400.



Figure 3: Power Curves - DGP LS5, n = 400

The goal of DGP LS5 is to show potential gains in using h(Z) in V to target alternatives. Following the discussion in Section 4.3, the variant of the  $\chi^2$ -test with  $h(Z) = \sqrt{3} \exp(-Z^2/2) - \sqrt{3/2}$  which maximises the absolute linear dependence of  $\mathbb{E}[K(Z - Z^{\dagger})h(Z^{\dagger})|Z]$  on  $a(Z) := \mathbb{E}[U|Z]$  namely,  $\chi^2_{AV}$ , is introduced. Including the "default"  $\chi^2$ -test which is agnostic about the alternative helps to visualize the power gains from targeting the alternative. One observes power gains relative to the bootstrap-based procedures. Thus, there are power gains to using the  $\chi^2$ -test when the researcher has an alternative in mind.<sup>5</sup>

The  $\chi^2$ -test is thus especially useful when the researcher has certain alternatives in mind (due to the adaptability of h(Z) to target alternatives), and when the researcher has a preference for a measure of correct model specification or mean independence without a formal hypothesis test (thanks to the pivotality of the test statistic). In sum, the simulations show that the proposed  $\chi^2$ -test, besides the easier interpretability that it offers relative to bootstrap-based ICM specification tests, has good size control and comparable power performance.

<sup>&</sup>lt;sup>5</sup>One such example is the linear versus quadratic first-stage IV specifications considered in Dieterle and Snell (2016).

#### 6.3 Running Time

An added advantage of a pivotal test is its computational efficiency vis-à-vis bootstrap-based procedures. This becomes essential, especially in large samples. Comparing the running times of competing tests is therefore in order. Table 6.3 compares the running times of the proposed pivotal  $\chi^2$ -test to the bootstrap-based ICM tests.<sup>6</sup>

	Average	e Runnin	g Time (s	seconds)	Median Relative Time					
n	$\chi^2$	Gauss	S&Z	Esc6	Gauss	S&Z	Esc6			
200	0.005	2.090	2.073	2.213	506.250	503.000	544.875			
	(0.002)	(0.132)	(0.134)	(0.142)	(328.583)	(322.833)	(346.375)			
400	0.011	2.184	2.165	2.961	238.222	239.444	324.222			
	(0.003)	(0.041)	(0.046)	(0.085)	(87.004)	(94.857)	(134.433)			
600	0.022	2.489	2.523	4.980	129.921	133.211	261.289			
	(0.005)	(0.036)	(0.076)	(0.035)	(46.358)	(52.096)	(95.995)			
800	0.039	2.909	2.914	8.721	84.159	83.479	254.721			
	(0.007)	(0.064)	(0.065)	(0.068)	(26.516)	(25.382)	(83.269)			

Table 6.3: Running Time - Specification Test - DGP LS1

Notes: The second row (in parentheses) for each sample size includes standard deviations and inter-quartile ranges for the average running times and relative times (with the  $\chi^2$ -test as the benchmark), respectively.

Table 6.3 shows clear computational gains of using the  $\chi^2$  specification test. The average running times of the  $\chi^2$ -test are negligible in comparison to the bootstrap-based procedures for all the sample sizes considered. One observes a striking difference in terms of median relative computational time. Although the median relative computational time of the other bootstrap-based procedures appears to decrease with the sample size, the computational gain remains considerable.

# 7 Conclusion

In spite of the 40-year-long history of ICM tests dating back to Bierens (1982), which has seen interesting contributions, a *bona fide* pivotalized ICM specification test remains lacking. This paper

<sup>&</sup>lt;sup>6</sup>All computations were carried out on a 2.8 GHz, Quad-Core Intel Core i7, and 16 GB MacBook Pro computer.

achieves the objective of proposing an omnibus  $\chi^2$  specification test and test of mean independence based on ICM metrics.

The proposed test solves a major drawback of ICM tests, where, the test statistic can be constructed with functional forms that boost power in the direction of alternatives the researcher may have in mind. The test is computationally more efficient than bootstrap-based procedures and remains viable even in large samples. In addition to providing a reliable pivotal test that draws its omnibus property from ICM metrics, the test statistic provides an easily interpretable metric of model specification and mean dependence that obviates formal hypothesis tests. The proposed test complements existing ICM specification tests as they are more clearly valuable in large samples where bootstrap-based procedures are computationally prohibitive or in cases where the researcher has certain alternatives in mind.

We conclude by highlighting several intriguing extensions to the current paper. This paper offers a viable solution for pivotalizing the ICM metrics. However, it is noteworthy that this solution necessitates regularization under the null hypothesis to address the ill-posed inverse problem. Exploring alternative formulations of V may offer solutions with more desirable theoretical properties. Moreover, we focus on the fixed-dimensional setting, and an extension to the high-dimensional setting would be an interesting topic. For instance, incorporating the projection idea proposed by Tan and Zhu (2022) and Sant'Anna and Song (2019) could be beneficial in handling models estimated via the LASSO. It would also be interesting to extend the idea to time series data, clustered data, and multiple-equation models with (non)-smooth objective functions. We leave these topics for future research.

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### Supplementary Material

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The supplementary material contains all technical proofs and additional simulation results. Section S.1 provides the proofs of theoretical results given in the main text. Section S.2 studies the asymptotic properties of the  $\chi^2$ -test based on  $\delta_V^*$ . Details on the GMDD metric developed in the main text are available in Section S.3, and Section S.4 discusses the relation between the proposed  $\chi^2$ -test and the family of CM tests. Section S.5 contains simulation results on mean independence tests. Section S.6 concludes with details of the numerical computation of the Bahadur slopes in Section 4.3.

To simplify notation, we use  $\mu_W := \mathbb{E}[W]$ ,  $\widetilde{W} := W - \mathbb{E}[W]$ ,  $\mu_W(Z) := \mathbb{E}[W|Z]$ ,  $\mathbb{E}_n[W] := n^{-1} \sum_{i=1}^n W_i$  throughout the supplement.

# S.1 Technical Proofs

### S.1.1 Proof of Proposition 2.1

- (1) The first part is similar to the proof of Theorem 4 in Li et al. (2023).
- (2) By simple algebra, we have

$$\begin{aligned} \operatorname{GMDD}_n(U|Z) &:= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} K(Z_i - Z_j) (U_i - \mathbb{E}_n[U]) (U_j - \mathbb{E}_n[U]) \\ &= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} K(Z_i - Z_j) (\widetilde{U}_i - \mathbb{E}_n[\widetilde{U}]) (\widetilde{U}_j - \mathbb{E}_n[\widetilde{U}]) \\ &= \frac{1}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \widetilde{U}_i \widetilde{U}_j + \frac{1}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \mathbb{E}_n[\widetilde{U}] \mathbb{E}_n[\widetilde{U}] \\ &\quad - \frac{2}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \widetilde{U}_i \mathbb{E}_n[\widetilde{U}] \\ &:= \sum_{k=1}^3 G_k \end{aligned}$$

The first summand is a second-order U-statistic. Let  $h(D_i, D_j) := K(Z_i - Z_j)\tilde{U}_i\tilde{U}_j$ , and  $h^{(1)}(D_i) = \mathbb{E}[h(D_i, D_j)|D_i]$ , then by the Hoeffding decomposition, we have

$$G_{1} = \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j}) \widetilde{U}_{i} \widetilde{U}_{j}$$

$$= \binom{n}{2}^{-1} \sum_{i < j}^{n} K(Z_{i} - Z_{j}) \widetilde{U}_{i} \widetilde{U}_{j}$$

$$= \text{GMDD}(U|Z) + \frac{2}{n} \sum_{i=1}^{n} [h^{(1)}(D_{i}) - \text{GMDD}(U|Z)] \qquad (S.125)$$

$$+ \frac{2}{n(n-1)} \sum_{i < j}^{n} [h(D_{i}, D_{j}) - h^{(1)}(D_{i}) - h^{(1)}(D_{j}) + \text{GMDD}(U|Z)].$$

$$= \text{GMDD}(U|Z) + \frac{2}{n} \sum_{i=1}^{n} [h^{(1)}(D_{i}) - \text{GMDD}(U|Z)] + o_{p}(n^{-1/2}),$$

by Theorem 3 in section 1.3 of Lee (1990).

By the Lindberg-Lévy Central Limit Theorem,  $\mathbb{E}_n[\tilde{U}] = O_p(n^{-1/2})$ . Thus, the second summand  $G_2$  is of order  $O_p(n^{-1})$ .

For the third summand, note that by the law of large numbers for U-statistics, we have

$$\frac{2}{n(n-1)} \sum_{i \neq j}^{n} K(Z_i - Z_j) \widetilde{U}_i = {\binom{n}{2}}^{-1} \sum_{i < j}^{n} K(Z_i - Z_j) (\widetilde{U}_i + \widetilde{U}_j) \xrightarrow{p} 2\mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}].$$

Hence,  $G_3 = -2\mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}](\mathbb{E}_n[\widetilde{U}]) + o_p(n^{-1/2}).$ 

Thus, by combining all the above terms, we have that

$$\sqrt{n}[\mathrm{GMDD}_n(U|Z) - \mathrm{GMDD}(U|Z)] = \frac{2}{\sqrt{n}} \sum_{i=1}^n \left\{ [h^{(1)}(D_i) - \mathrm{GMDD}(U|Z)] - \mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}]\widetilde{U}_i \right\} + o_p(1).$$

The result follows from the Lindberg-Lévy Central Limit Theorem.

### S.1.2 Proof of Lemma 3.2

For  $V = [h(Z), U - h(Z)]^{\top}$  in Lemma 3.1,

$$\begin{split} \delta_V^* &= \left[ \mathbb{E}[\widetilde{U}^{\dagger}\widetilde{h}(Z)K(Z-Z^{\dagger})], \ -\mathrm{GMDD}(U|Z) - \mathbb{E}[\widetilde{U}^{\dagger}\widetilde{h}(Z)K(Z-Z^{\dagger})] \right]^{\top} \\ &- \left[ \mathbb{E}[h(Z)]\mu_U, \ \mu_U^2 - \mathbb{E}[h(Z)]\mu_U \right]^{\top} \mathbb{E}[K(Z-Z^{\dagger})] \\ &= \left[ \mathbb{E}[\widetilde{U}^{\dagger}\widetilde{h}(Z)K(Z-Z^{\dagger})] - \mathbb{E}[K(Z-Z^{\dagger})]\mathbb{E}[h(Z)]\mu_U, \\ &- \mathrm{GMDD}(U|Z) - \mathbb{E}[\widetilde{U}^{\dagger}\widetilde{h}(Z)K(Z-Z^{\dagger})] - \mathbb{E}[K(Z-Z^{\dagger})](\mu_U^2 - \mathbb{E}[h(Z)]\mu_U) \right]^{\top} \\ &:= [\delta_V^{*(1)}, \ \delta_V^{*(2)}]^{\top}. \end{split}$$

Thus,

$$\delta_V^{*(1)} + \delta_V^{*(2)} = -\text{GMDD}(U|Z) - \mu_U^2 \mathbb{E}[K(Z - Z^{\dagger})].$$

If  $\mu_U(Z) = 0$ , then  $\mu_U = 0$  by the LIE. This implies that  $\delta_V^* = 0$ .

Conversely, if  $\delta_V^* = 0$ , then we must have  $\delta_V^{*(1)} + \delta_V^{*(2)} = 0$ . Note that both -GMDD(U|Z) and  $-\mu_U^2 \mathbb{E}[K(Z - Z^{\dagger})]$  are non-negative, thus we must have GMDD(U|Z) = 0 and  $\mu_U^2 \mathbb{E}[K(Z - Z^{\dagger})] = 0$ , corresponding to  $\mu_U(Z) = \mu_U$  and  $\mu_U = 0$ , respectively. Hence  $\mu_U(Z) = 0$ .

# S.1.3 Proof of Theorem 4.1

We first decompose  $\widehat{\delta}_V$  into four summands,

$$\begin{split} \widehat{\delta}_{V} &:= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} K(Z_{i} - Z_{j})(V_{i} - \mathbb{E}_{n}[V])(U_{j} - \mathbb{E}_{n}[U]) \\ &= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} K(Z_{i} - Z_{j})(\widetilde{V}_{i} - \mathbb{E}_{n}[\widetilde{V}])(\widetilde{U}_{j} - \mathbb{E}_{n}[\widetilde{U}]) \\ &= \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j})\widetilde{V}_{i}\widetilde{U}_{j} + \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j})\mathbb{E}_{n}[\widetilde{V}]\mathbb{E}_{n}[\widetilde{U}] \\ &- \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j})\widetilde{V}_{i}\mathbb{E}_{n}[\widetilde{U}] - \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j})\widetilde{U}_{i}\mathbb{E}_{n}[\widetilde{V}] \\ &= : \sum_{k=1}^{4} \widehat{\delta}_{V,k}. \end{split}$$
(S.126)

The first summand is a second-order U-statistic. Let  $\psi(D_i, D_j) := K(Z_i - Z_j)(\widetilde{V}_i \widetilde{U}_j + \widetilde{V}_j \widetilde{U}_i)$ , and  $\psi^{(1)}(D_i) = \mathbb{E}[\psi(D_i, D_j)|D_i]$ , then by the Hoeffding decomposition, we have

$$\begin{split} \widehat{\delta}_{V,1} &= \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_i - Z_j) \widetilde{V}_i \widetilde{U}_j \\ &= \binom{n}{2}^{-1} \sum_{i < j}^{n} K(Z_i - Z_j) (\widetilde{V}_i \widetilde{U}_j + \widetilde{V}_j \widetilde{U}_i) / 2 \\ &= \delta_V + \frac{1}{n} \sum_{i=1}^{n} [\psi^{(1)}(D_i) - 2\delta_V] + \frac{1}{n(n-1)} \sum_{i < j}^{n} [\psi(D_i, D_j) - \psi^{(1)}(D_i) - \psi^{(1)}(D_j) + 2\delta_V]. \end{split}$$
(S.127)  
$$&= \delta_V + \frac{1}{n} \sum_{i=1}^{n} [\psi^{(1)}(D_i) - 2\delta_V] + o_p(n^{-1/2}), \end{split}$$

where the last equality holds by Theorem 3 in section 1.3 of Lee (1990). Here, we also note that

$$\psi^{(1)}(D_i) = \mathbb{E}[\psi(D_i, D_j) | D_i] = \left\{ \mathbb{E}[K(Z_i - Z_j) \widetilde{V}_j \widetilde{U}_i | D_i] + \mathbb{E}[K(Z_i - Z_j) \widetilde{V}_i \widetilde{U}_j | D_i] \right\}$$
  
$$:= \left\{ m_{\widetilde{V}}(Z_i) \widetilde{U}_i + m_{\widetilde{U}}(Z_i) \widetilde{V}_i \right\},$$
 (S.128)

where  $m_{\widetilde{U}}(Z) = \mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}^{\dagger}|Z]$ , and  $m_{\widetilde{V}}(Z) = \mathbb{E}[K(Z - Z^{\dagger})\widetilde{V}^{\dagger}|Z]$ .

By the Lindberg-Lévy Central Limit Theorem,  $\mathbb{E}_n[\widetilde{U}] = O_p(n^{-1/2})$  and  $\mathbb{E}_n[\widetilde{V}] = O_p(n^{-1/2})$ . Thus, the second summand  $\widehat{\delta}_{V,2}$  is of order  $O_p(n^{-1})$ .

For the third and fourth summands, note that by the law of large numbers for U-statistics, we have

$$\frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_i - Z_j) \widetilde{V}_i = {\binom{n}{2}}^{-1} \sum_{i < j}^{n} K(Z_i - Z_j) (\widetilde{V}_i + \widetilde{V}_j)/2$$
$$\xrightarrow{p} \mathbb{E}[K(Z - Z^{\dagger}) \widetilde{V}] := \mathbb{E}[m_{\widetilde{V}}(Z)].$$

Similarly,

$$\frac{1}{n(n-1)}\sum_{i\neq j}^{n} K(Z_i - Z_j)\widetilde{U}_i \xrightarrow{p} \mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}] := \mathbb{E}[m_{\widetilde{U}}(Z)].$$

Hence,  $\widehat{\delta}_{V,3} = -\mathbb{E}[m_{\widetilde{V}}(Z)](\mathbb{E}_n[\widetilde{U}]) + o_p(n^{-1/2})$ , and  $\widehat{\delta}_{V,4} = -\mathbb{E}[m_{\widetilde{U}}(Z)]\mathbb{E}_n[\widetilde{V}] + o_p(n^{-1/2})$ .

Thus, combining all all above terms, together with (S.126), (S.128) and (S.127), we obtain

$$\widehat{\delta}_{V} = \delta_{V} + \frac{1}{n} \sum_{i=1}^{n} \left\{ m_{\widetilde{V}}(Z_{i}) - \mathbb{E}[m_{\widetilde{V}}(Z)] \right\} \widetilde{U}_{i} - \delta_{V} + \frac{1}{n} \sum_{i=1}^{n} \left\{ m_{\widetilde{U}}(Z_{i}) - \mathbb{E}[m_{\widetilde{U}}(Z)] \right\} \widetilde{V}_{i} - \delta_{V} + o_{p}(n^{-1/2}).$$
(S.129)

(i) Under  $\mathbb{H}_o$ , we have  $\delta_V = 0$ , and

$$m_{\widetilde{U}}(Z) = \mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}^{\dagger}|Z] = \mathbb{E}\{K(Z - Z^{\dagger})\mathbb{E}[\widetilde{U}^{\dagger}|Z, Z^{\dagger}]|Z\} = 0 \ a.s.$$

This also implies that  $\mathbb{E}[m_{\widetilde{U}}(Z)] = 0$  under  $\mathbb{H}_o$ , and hence using (S.129),

$$\sqrt{n}\widehat{\delta}_V = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i) - \mathbb{E}[m_{\widetilde{V}}(Z)] \right\} \widetilde{U}_i + o_p(1).$$

Asymptotic normality thus follows from Assumption 4.1 and the Lindberg-Lévy Central Limit Theorem.

(ii) Under  $\mathbb{H}'_{an}$ , we have

$$\delta_V = \mathbb{E}[K(Z - Z^{\dagger})\widetilde{U}^{\dagger}\widetilde{V}] = \mathbb{E}\left[\mathbb{E}[\widetilde{U}^{\dagger}|Z^{\dagger}]K(Z - Z^{\dagger})\widetilde{V}\right] = n^{-1/2}\mathbb{E}\left[a(Z^{\dagger})K(Z - Z^{\dagger})\widetilde{V}\right] = n^{-1/2}a_o,$$

by the independence between D = (U, V, Z) and  $D^{\dagger} = (U^{\dagger}, V^{\dagger}, Z^{\dagger})$  and the LIE.

Furthermore, we have that  $m_{\widetilde{U}}(Z) = \mathbb{E}\{K(Z-Z^{\dagger})\mathbb{E}(\widetilde{U}^{\dagger}|Z^{\dagger},Z)]|Z\} = \frac{1}{\sqrt{n}}\mathbb{E}[K(Z-Z^{\dagger})a(Z^{\dagger})|Z]$ . Hence by the law of large numbers,

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ m_{\widetilde{U}}(Z_i) - \mathbb{E}[m_{\widetilde{U}}(Z)] \right\} \widetilde{V}_i - \sqrt{n} \delta_V$$
  
$$= \frac{1}{n} \sum_{i=1}^{n} \left\{ \mathbb{E}[K(Z_i - Z^{\dagger})a(Z^{\dagger})|Z_i] - \mathbb{E}[K(Z - Z^{\dagger})a(Z^{\dagger})] \right\} \widetilde{V}_i - \sqrt{n} \delta_V$$
  
$$\Rightarrow_p \mathbb{E}\{\mathbb{E}[K(Z - Z^{\dagger})a(Z^{\dagger})|Z] \widetilde{V}\} - \mathbb{E}[K(Z - Z^{\dagger})a(Z^{\dagger})] \mathbb{E} \widetilde{V} - a_0 = a_0 - 0 - a_0 = 0.$$

Therefore, by (S.129), we obtain that

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$$\sqrt{n}(\widehat{\delta}_V - \delta_V) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i)\widetilde{U}_i - \mathbb{E}[m_{\widetilde{V}}(Z)]\widetilde{U}_i - \delta_V \right\} + o_p(1).$$

Under  $\mathbb{H}'_{an}$ ,  $\mathbb{E}\left\{m_{\widetilde{V}}(Z_i)\widetilde{U}_i - \mathbb{E}[m_{\widetilde{V}}(Z)]\widetilde{U}_i - \delta_V\right\} = 0$ , hence the asymptotic normality follows. Furthermore, since  $\delta_V = O(n^{-1/2})$ , it can be shown that

$$\operatorname{Var}(\phi(D_i)) - \Omega_{V_o} = O(n^{-1/2}),$$

and the continuous mapping theorem applies.

(iii) Note that  $\delta_V \neq 0$  under  $\mathbb{H}_a$ , the result follows directly from (S.129).

#### S.1.4 Proof of Theorem 4.2

By Theorem 2, equation (3.3) in Maesono (1998), we know that

$$\widetilde{\Omega}_{V,n} - \Omega_V = O_p(n^{-1/2}),$$

for both  $\mathbb{H}_o$  and  $\mathbb{H}'_a$ . Furthermore, under  $\mathbb{H}'_{an}$ , we know that  $\Omega_V - \Omega_{V_o} = O(n^{-1/2})$ . Hence, for any small  $\iota \in (0, 1/2), n^{1/2-\iota}(\widetilde{\Omega}_{V,n} - \Omega_{V_o}) = o_p(1)$ , under  $\mathbb{H}_o$  and  $\mathbb{H}'_{an}$ . This implies that Assumption 2.2 in Dufour and Valéry (2016) holds by setting  $b_n = n^{1/2}$  and  $c_n = Cn^{-1/2+\iota}$  for some constant C > 0. Furthermore, by Proposition 9.1 in Dufour and Valéry (2016), we know that  $\widehat{\Omega}_{V,n}^- \xrightarrow{p} \Omega_{V_o}^-$  under  $\mathbb{H}_o$  and  $\mathbb{H}'_{an}$ . Similarly,  $\widehat{\Omega}_{V,n}^- \xrightarrow{p} \Omega_{V_a}^-$  under  $\mathbb{H}'_a$ .

- (i). By Corollary 9.3 in Dufour and Valéry (2016),  $T_{V,n} \xrightarrow{d} \chi^2_{\operatorname{rank}(\Omega_{V_0})}$ .
- (ii). By the continuous mapping theorem and theorem 4.1 (ii),

$$T_{V,n} \xrightarrow{d} \chi^2_{\operatorname{rank}(\Omega_{V_o})}(\theta).$$

(iii). When  $\delta_V \notin \mathcal{M}_0$ , we have that  $\lim_{n \to \infty} T_{V,n} = \lim_{n \to \infty} n \delta_V^\top \Omega_{V_a}^- \delta_V = \infty$ , in probability, and the result follows.

### S.1.5 Proof of the Result in Remark 4.3

**Lemma S.1.1.**  $\delta_V \notin \mathcal{M}_0$  for V in Lemma 3.1.

*Proof.* Under  $\mathbb{H}'_a$ , we have  $\mathbb{E}[U|Z] - \mathbb{E}[U] = a(Z)$  with  $\mathbb{E}a(Z) = 0$ . Define  $\tilde{h}(Z) = h(Z) - \mathbb{E}[h(Z)]$ . Then

$$m_{\widetilde{V}}(Z) = \left[ \mathbb{E}\{K(Z - Z^{\dagger})\widetilde{h}(Z^{\dagger})|Z\}, \ \mathbb{E}\{K(Z - Z^{\dagger})[a(Z^{\dagger}) - \widetilde{h}(Z^{\dagger})]|Z\} \right]^{\top} \text{ and } m_{\widetilde{U}}(Z) = \mathbb{E}\{K(Z - Z^{\dagger})a(Z^{\dagger})|Z\}.$$

First, when  $\Omega_a$  is of rank 2, the claim holds because  $\delta_V \neq \mathbf{0}^{\top}$  under  $\mathbb{H}'_a$ .

Second, recall that  $\Omega_a = \operatorname{Var}\{\phi(D)\}$  with  $\phi(D) = [m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)](V - \mathbb{E}V) + [m_{\widetilde{V}}(Z) - \mathbb{E}m_{\widetilde{V}}(Z)](U - \mathbb{E}U)$  and  $\Omega_V = \operatorname{Var}\{\phi(D)\}$ . By the Cauchy-Schwarz inequality, we know that  $\Omega_a$  is of rank one if and

only if for some constant  $C \neq -1$ ,

$$\phi(D)^{\top}[-C,1] = 0 \ a.s.$$

Here we rule out C = -1 as it indicates that GMDD(a(Z)|Z) = 0, a contradiction of  $\mathbb{H}'_a$ .

Let  $f(Z^{\dagger}) := a(Z^{\dagger}) - (C+1)\widetilde{h}(Z^{\dagger})$ , this implies that

$$[m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)][\widetilde{U} - (C+1)\widetilde{h}(Z)] + [m_{\widetilde{f}}(Z) - \mathbb{E}m_{\widetilde{f}}(Z)]\widetilde{U} = 0 \ a.s.$$
(S.130)

where  $m_{\widetilde{U}}(Z) = \mathbb{E}\{K(Z-Z^{\dagger})\widetilde{U}^{\dagger}|Z\}$ , and  $m_{\widetilde{f}}(Z) = \mathbb{E}\{K(Z-Z^{\dagger})f(Z^{\dagger})|Z\}$ .

Recall that  $\mathbb{E}[\widetilde{U}|Z] = a(Z)$ , by taking conditional expectation of (S.130) w.r.t. Z, we have

$$[m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)]f(Z) + [m_{\widetilde{f}}(Z) - \mathbb{E}m_{\widetilde{f}}(Z)]a(Z) = 0 \ a.s.$$
(S.131)

Therefore, by taking the difference, we have

$$\left\{m_{\widetilde{U}}(Z) + m_{\widetilde{f}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z) + \mathbb{E}m_{\widetilde{f}}(Z)\right\} [\widetilde{U} - a(Z)] = 0 \ a.s.$$

In light of the foregoing, either one of the following holds:

- (1)  $\widetilde{U} = a(Z) \ a.s.$
- (2)  $\widetilde{U} \neq a(Z)$ , so that the coefficient on  $\widetilde{U}$  in (S.130) is zero, i.e.

$$\left\{m_{\widetilde{U}}(Z) + m_{\widetilde{f}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z) + \mathbb{E}m_{\widetilde{f}}(Z)\right\} = 0 \ a.s.$$

which further implies that  $[m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)]\widetilde{h}(Z) = 0$  a.s. in combination of (S.130). We proceed using proof by contradiction.

If (1) holds, we have

$$\Omega_a = \operatorname{Var}\left\{ [m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)]h(Z) + [m_{\widetilde{h}}(Z) - \mathbb{E}m_{\widetilde{h}}(Z)]a(Z)|D] \right\} \begin{bmatrix} 1 & C \\ C & C^2 \end{bmatrix}$$

which implies  $\mathcal{M}_0 = \{(x, y)^\top | x = -Cy, y \in \mathbb{R}\}$ . Note in this case, by taking the expectation of (S.131), we can show that  $\mathbb{E}\{K(Z - Z^{\dagger})a(Z^{\dagger})[a(Z) - \tilde{h}(Z)]\} = C\mathbb{E}[K(Z - Z^{\dagger})a(Z^{\dagger})h(Z)]$ , so that  $\delta_V = \mathbb{E}[K(Z - Z^{\dagger})a(Z^{\dagger})h(Z)][1, C]^\top \notin \mathcal{M}_0$ .

If (2) holds, then we have  $m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z) = 0$  a.s. since  $\widetilde{h}(Z)$  is non-degenerate. This implies that  $\mathbb{E}\{[m_{\widetilde{U}}(Z) - \mathbb{E}m_{\widetilde{U}}(Z)]a(Z)\} = \text{GMDD}(U|Z) = 0$ , a contradiction.

### S.1.6 Proof of Theorem 4.3

For two functions  $f_a(x)$  and  $f_b(x)$ , write  $f_a(x) \sim f_b(x)$  if and only if  $f_a(x)/f_b(x) \to 1$  as  $x \to \infty$ . By Zolotarev (1961), we know that

$$\log \mathbb{P}\Big(\sum_{k=1}^{\infty} \lambda_k G_k^2 > x\Big) \sim -x/(2\lambda_1), \quad \text{as } x \to \infty.$$

Clearly, under  $\mathbb{H}'_a$ , we have  $n \text{GMDD}_n(U|Z) \to \infty$  in probability. Thus,

$$c_G = \underset{n \to \infty}{\text{plim}} \frac{n \text{GMDD}_n(U|Z)}{n\lambda_1} = \frac{\text{GMDD}(U|Z)}{\lambda_1},$$

where we note that  $\text{GMDD}_n(U|Z) \to_{a.s.} \text{GMDD}(U|Z)$ . The first result holds by noting  $\text{GMDD}(U|Z) = -\mathbb{E}[a(Z)a(Z^{\dagger})K(Z-Z^{\dagger})].$ 

Next, by the large deviation result for the chi-squared distribution,

$$\log \mathbb{P}(\chi^2_{\operatorname{rank}(\Omega_{V_o})} > x) \sim -x/2 \quad \text{as } x \to \infty.$$

Recall  $a_o = \mathbb{E}[(\mu_V(Z) - \mu_V)a(Z^{\dagger})K(Z - Z^{\dagger})]$  and  $\lim_{n \to \infty} T_{V,n} = \lim_{n \to \infty} na_o^{\top} \Omega_{V_a}^{-} a_o = \infty$  under  $\mathbb{H}'_a$ , thus

$$c_T = \lim_{n \to \infty} \frac{2}{n} \frac{n a_o^\top \Omega_{V_a}^- a_o}{2} = a_o^\top \Omega_{V_a}^- a_o.$$

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### S.1.7 Proof of Theorem 5.1

Define  $r_i := \partial g(X_i; \beta_o) / \partial \beta_o \in \mathbb{R}^k$ , then under Condition 5.2, we can obtain

$$\widehat{U}_{i} = Y_{i} - g(X_{i};\widehat{\beta}_{n}) = \mathcal{E}_{i} + n^{-1/2}a(X_{i}, Z_{i}) + g(X_{i};\beta_{o}) - g(X_{i};\widehat{\beta}_{n}) 
= \mathcal{E}_{i} + n^{-1/2}a(X_{i}, Z_{i}) - r_{i}^{\top}(\widehat{\beta}_{n} - \beta_{o}) + o_{p}(n^{-1/2})$$
(S.132)

by Taylor expansion.

By Condition 5.3, we know that  $\hat{\beta}_n - \beta_o = O_p(n^{-1/2})$ . Then, rewriting  $\hat{V}_i = V_i + \hat{V}_i - V_i$  and  $\hat{U}_i = \mathcal{E}_i + \hat{U}_i - \mathcal{E}_i$ , the symmetrized U-statistic estimator is given by

$$\begin{split} \widehat{\delta}_{n} &= \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ \widehat{V}_{j} \widehat{U}_{i} + \widehat{V}_{i} \widehat{U}_{j} \right] \\ &= \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ (V_{j} + \widehat{V}_{j} - V_{j}) (\mathcal{E}_{i} + \widehat{U}_{i} - \mathcal{E}_{i}) + (V_{i} + \widehat{V}_{i} - V_{i}) (\mathcal{E}_{j} + \widehat{U}_{j} - \mathcal{E}_{j}) \right] \\ &= \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ V_{i} \mathcal{E}_{j} + V_{j} \mathcal{E}_{i} \right] + \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ \mathcal{E}_{i} \xi_{j}^{\top} + \mathcal{E}_{j} \xi_{i}^{\top} \right] (\widehat{\beta}_{n} - \beta_{o}) \\ &+ \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ V_{j} n^{-1/2} a(X_{i}, Z_{i}) + V_{i} n^{-1/2} a(X_{j}, Z_{j}) \right] \\ &- \frac{1}{n(n-1)} \sum_{i < j} K(Z_{i} - Z_{j}) \left[ V_{j} r_{i}^{\top} + V_{i} r_{j}^{\top} \right] (\widehat{\beta}_{n} - \beta_{o}) + o_{p} (n^{-1/2}) \\ &:= R_{n1} + R_{n2} + R_{n3} + R_{n4} + o_{p} (1), \end{split}$$

where the third equality holds by Condition 5.4 (i) and (S.132).

By arguments similar to those in the proof of Theorem 4.1,

$$\sqrt{n}R_{n1} = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\psi^{(1)}(D_i) + o_p(1)$$

with  $U_i$  replaced with  $\mathcal{E}_i$ . Furthermore, by the law of large numbers for U-statistics and Condition 5.3(i),

$$\sqrt{n}(R_{n2} + R_{n4}) = \frac{1}{n(n-1)} \sum_{i < j} K(Z_i - Z_j) (\mathcal{E}_i \xi_j^\top + \mathcal{E}_j \xi_i^\top - V_j r_i^\top - V_i r_j^\top) \sqrt{n} (\hat{\beta}_n - \beta_o) \\
= \left(\Xi_1 + o_p(1)\right) \left(\zeta_a + \frac{1}{\sqrt{n}} \sum_{i=1}^n \varphi_i \mathcal{E}_i + o_p(1)\right),$$

where we note that  $\mathbb{E}[K(Z_i - Z_j)\mathcal{E}_i\xi_j^{\top}] = 0$  by the fact that  $\mathbb{E}[\mathcal{E}_i|Z_i] = 0$  and LIE.

Similarly, the law of large numbers for U-statistics implies

$$\sqrt{n}R_{n3} = \mathbb{E}[K(Z_i - Z_j)a(X_i, Z_i)V_j] + o_p(1).$$

Thus, Slutsky's theorem implies

$$\sqrt{n}\widehat{\delta}_n = \Xi_a + \Xi_1\zeta_a + \frac{1}{\sqrt{n}} \Big(\sum_{i=1}^n \psi^{(1)}(D_i) + \Xi_1\sum_{i=1}^n \varphi_i \mathcal{E}_i\Big) + o_p(1) \xrightarrow{d} \mathcal{N}(\Xi_a + \Xi_1\zeta_a, \ \Omega_\delta)$$

with

$$\Omega_{\delta} = \Omega_{V} + \Xi_{1} \mathbb{E}[\varphi_{i} \varphi_{i}^{\top} \mathcal{E}_{i}^{2}] \Xi_{1}^{\top} + \Xi_{1} \mathbb{E}[\varphi_{i} \mathcal{E}_{i} \psi^{(1)}(D_{i})^{\top}] + \mathbb{E}[\psi^{(1)}(D_{i}) \mathcal{E}_{i} \varphi_{i}^{\top}] \Xi_{1}^{\top}.$$

### S.1.8 Proof of Lemma 5.1

From the proof of Theorem 5.1, we know that under  $\mathbb{H}_o$ 

$$\sqrt{n}\widehat{\delta}_{n} = \frac{1}{\sqrt{n}} \Big( \sum_{i=1}^{n} \psi^{(1)}(D_{i}) + \Xi_{1} \sum_{i=1}^{n} \varphi_{i}U_{i} \Big) + o_{p}(1) \\
= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (m_{V}(Z_{i}) + \Xi_{1}\varphi_{i})U_{i} + o_{p}(1) \\
= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (m_{V}(Z_{i}) - \mathbb{E}[m_{V}(Z)r^{\top}]\varphi_{i})U_{i} + o_{p}(1) \\
= [1, -1]^{\top} \times \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (m_{h}(Z_{i}) - \mathbb{E}[m_{h}(Z)r^{\top}]\varphi_{i})U_{i} + o_{p}(1)$$
(S.133)

where  $\psi^{(1)}(D_i) = m_V(Z_i)U_i$ ,  $m_V(Z) := \mathbb{E}[K(Z - Z^{\dagger})V^{\dagger}|Z]$ , and  $\Xi_1 = \mathbb{E}[K(Z - Z^{\dagger})(U\xi^{\dagger \top} - V^{\dagger}r^{\top})] = -\mathbb{E}[K(Z - Z^{\dagger})V^{\dagger}r^{\top}] = -\mathbb{E}[m_V(Z)r^{\top}]$  noting that  $\mathbb{E}[U|D^{\dagger}, Z] = \mathbb{E}[U|Z] = 0$  a.s. under  $\mathbb{H}_o$ . For V of the form  $[h(Z), U - h(Z)]^{\top}$  under  $\mathbb{H}_o$ ,  $m_V(Z) = [1, -1]^{\top} \times m_h(Z)$  where  $m_h(Z) := \mathbb{E}[K(Z - Z^{\dagger})h(Z^{\dagger})|Z]$ ; the last equality hence follows. The result follows because the leading term in (S.133) is the product of  $[1, -1]^{\top}$  and a non-degenerate scalar-valued random variable.

# **S.2** Asymptotic properties of $\hat{\delta}_V^*$ .

When one is interested in the testing (12), a natural empirical estimator for  $\delta_V^*$  is given by

$$\widehat{\delta}_V^* = \widehat{\delta}_V - \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} K(Z_i - Z_j) \mathbb{E}_n U \mathbb{E}_n V.$$

To analyze the asymptotic behavior of  $\hat{\delta}_V^*$ , we further consider the following local and fixed alternatives:

$$\mathbb{H}_{an}^*: \mathbb{E}[U|Z] = n^{-1/2}a(Z) \text{ and } \mathbb{H}_a^*: \mathbb{E}[U|Z] = a(Z),$$

where a(Z) is a non-degenerate measurable function of Z (not necessarily mean zero). Let  $m_U(Z) = \mathbb{E}[K(Z - Z^{\dagger})U^{\dagger}|Z], m_V(Z) = \mathbb{E}[K(Z - Z^{\dagger})V^{\dagger}|Z], \widetilde{K}(Z) = \mathbb{E}[K(Z - Z^{\dagger})|Z] - \mathbb{E}[K(Z - Z^{\dagger})],$  and

$$\phi^*(D) = \left\{ m_{\widetilde{V}}(Z) - \mathbb{E}[m_V(Z)] \right\} (U - \mathbb{E}U) + \left\{ m_{\widetilde{U}}(Z) - \mathbb{E}[m_U(Z)] \right\} (V - \mathbb{E}V) - 2\mathbb{E}U\mathbb{E}V\widetilde{K}(Z).$$

**Theorem S.2.1.** Let the conditions of Theorem 4.1 hold, then

- (i) under  $\mathbb{H}_{o}^{*}, \sqrt{n}\widehat{\delta}_{V}^{*} \xrightarrow{d} \mathcal{N}(0, \Omega_{V_{o}}^{*});$
- (ii) under  $\mathbb{H}_{an}^*$ ,  $\sqrt{n}\widehat{\delta}_V^* \xrightarrow{d} \mathcal{N}(a_o^*, \Omega_{V_o}^*)$ ; and
- (iii) under  $\mathbb{H}_a^*$ ;  $\sqrt{n}(\widehat{\delta}_V^* \delta_V^*) \xrightarrow{d} \mathcal{N}(0, \Omega_{V_a}^*)$ ,

where  $a_o^* := \mathbb{E}\{(V - \mathbb{E}V)[a(Z^{\dagger}) - \mathbb{E}a(Z)]K(Z - Z^{\dagger})\} - \mathbb{E}V\mathbb{E}a(Z)\mathbb{E}K(Z - Z^{\dagger}), \text{ and } \Omega_{V_o}^* \text{ and } \Omega_{V_a}^* \text{ correspond}$ to specific expressions of  $\Omega_V^* = \operatorname{Var}[\phi^*(D)]$  under  $\mathbb{H}_o^*$  and  $\mathbb{H}_a^*$ , respectively.

**Proof.** (i) Note that by the law of large numbers (for U-statistics), we have

$$\widehat{\delta}_{V}^{*} = \widehat{\delta}_{V} - \frac{1}{n(n-1)} \sum_{i \neq j}^{n} K(Z_{i} - Z_{j}) \mathbb{E}_{n}[V] \mathbb{E}_{n}[U]$$
$$= \widehat{\delta}_{V} - [\mathbb{E}K(Z_{i} - Z_{j}) \mathbb{E}V + o_{p}(1)] \mathbb{E}_{n}[U].$$

Under  $\mathbb{H}_{o}^{*}$ , we have  $U_{i} = \widetilde{U}_{i}$ . Therefore, by (S.129), we have

$$\widehat{\delta}_V^* = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i) - \mathbb{E}[m_V(Z)] \right\} U_i + o_p(1),$$

where  $\mathbb{E}[m_V(Z)] = \mathbb{E}[K(Z - Z^{\dagger})V^{\dagger}]$ . The result follows from the Lindberg-Lévy Central Limit Theorem. (ii) Under  $\mathbb{H}_{an}^*$ , we have  $\mathbb{E}U = n^{-1/2}\mathbb{E}[a(Z)]$ . In this case, we have

$$\sqrt{n}(\widehat{\delta}_V^* - \widehat{\delta}_V) = -[\mathbb{E}K(Z_i - Z_j)\mathbb{E}V + o_p(1)][\mathbb{E}a(Z_i) + \sqrt{n}\mathbb{E}_n\widetilde{U}_i].$$

Therefore, by (S.129) and the proof of Theorem 4.1 (ii), we have

$$\begin{split} &\sqrt{n}(\widehat{\delta}_V^* - \delta_V) \\ = &\frac{1}{\sqrt{n}} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i) \widetilde{U}_i - \mathbb{E}[m_{\widetilde{V}}(Z)] \widetilde{U}_i - \delta_V \right\} - \mathbb{E}K(Z_i - Z_j) \mathbb{E}V \mathbb{E}a(Z) - \sqrt{n} \mathbb{E}K(Z_i - Z_j) \mathbb{E}V \mathbb{E}n \widetilde{U}_i + o_p(1) \\ = &\frac{1}{\sqrt{n}} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i) \widetilde{U}_i - \mathbb{E}[m_V(Z)] \widetilde{U}_i - \delta_V \right\} - \mathbb{E}K(Z_i - Z_j) \mathbb{E}V \mathbb{E}a(Z) + o_p(1), \end{split}$$

where  $\delta_V = n^{-1/2} \mathbb{E} \left[ \widetilde{V} [a(Z^{\dagger}) - \mathbb{E} a(Z^{\dagger})] K(Z - Z^{\dagger}) \right].$ 

Therefore, we obtain that

$$\sqrt{n}\widehat{\delta}_V^* = \delta_V^* + \frac{1}{\sqrt{n}}\sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i)\widetilde{U}_i - \mathbb{E}[m_V(Z)]\widetilde{U}_i - \delta_V \right\} + o_p(1)$$

with  $\delta_V^* = \delta_V - \mathbb{E}K(Z_i - Z_j)\mathbb{E}V\mathbb{E}a(Z) = a_0^*$ .

(iii) Recalling  $\mathbb{E}_n U = \mathbb{E}U + \mathbb{E}_n \widetilde{U}$  and  $\mathbb{E}_n V = \mathbb{E}V + \mathbb{E}_n \widetilde{V}$ , we have

$$\begin{split} \sqrt{n}(\widehat{\delta}_V^* - \widehat{\delta}_V) &= -\frac{\sqrt{n}}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \mathbb{E}_n \widetilde{V} \mathbb{E}_n \widetilde{U} - \frac{\sqrt{n}}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \mathbb{E} V \mathbb{E}_n \widetilde{U} \\ &- \frac{\sqrt{n}}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \mathbb{E} U \mathbb{E}_n \widetilde{V} - \frac{\sqrt{n}}{n(n-1)} \sum_{i \neq j}^n K(Z_i - Z_j) \mathbb{E} U \mathbb{E} V \\ &:= -\sum_{k=1}^4 R_k. \end{split}$$

By the law of large numbers and the Lindberg-Lévy Central Limit Theorem, it is not hard to see that

$$R_1 = O_p(n^{-1/2}) = o_p(1), \quad R_2 = \sqrt{n} \mathbb{E}K(Z_i - Z_j) \mathbb{E}V \mathbb{E}_n \widetilde{U} + o_p(1), \quad R_3 = \sqrt{n} \mathbb{E}K(Z_i - Z_j) \mathbb{E}U \mathbb{E}_n \widetilde{V} + o_p(1).$$

Applying the Hoeffding decomposition to  $R_4$ , we have that

$$\sqrt{n}[R_4 - \mathbb{E}K(Z_i - Z_j)\mathbb{E}U\mathbb{E}V] = \frac{2}{\sqrt{n}}\sum_{i=1}^n \mathbb{E}U\mathbb{E}V\widetilde{K}_i + o_p(1),$$

where  $\widetilde{K}_i = \mathbb{E}[K(Z_i - Z_j)|Z_i] - \mathbb{E}K(Z_i - Z_j).$ 

Together with (S.129), we obtain that

$$\begin{split} \sqrt{n}(\widehat{\delta}_V^* - \delta_V^*) = &\frac{1}{n} \sum_{i=1}^n \left\{ m_{\widetilde{V}}(Z_i) - \mathbb{E}[m_V(Z)] \right\} \widetilde{U}_i - \delta_V + \frac{1}{n} \sum_{i=1}^n \left\{ m_{\widetilde{U}}(Z_i) - \mathbb{E}[m_U(Z)] \right\} \widetilde{V}_i - \delta_V \\ &- \frac{2}{\sqrt{n}} \sum_{i=1}^n \mathbb{E}U \mathbb{E}V \widetilde{K}_i + o_p(1), \end{split}$$

where  $\delta_V^* = \delta_V - \mathbb{E}K(Z - Z^{\dagger})\mathbb{E}a(Z)\mathbb{E}V] = a_0^*$ .

Also,

$$\Omega_{V_a}^* = \operatorname{Var}\left[\left\{m_{\widetilde{V}}(Z_i) - \mathbb{E}[m_V(Z)]\right\}\widetilde{U}_i + \left\{m_{\widetilde{U}}(Z_i) - \mathbb{E}[m_U(Z)]\right\}\widetilde{V}_i - 2\mathbb{E}U\mathbb{E}V\widetilde{K}_i\right].$$
(S.234)

### S.3 The GMDD Metric

Section S.3.1 discusses the class of suitable ICM integrating measures and Section S.3.2 provides a characterization and concrete examples of GMDD metrics.

### S.3.1 Integrating Measures

The measure  $\nu$  ought to be "suitable" in some sense for the resulting metric to be a valid ICM metric. The following proposition provides further clarification.

**Proposition S.3.1.** Let  $Z \in \mathbb{R}^{p_z}$  and  $U \in \mathbb{R}$  with  $\mathbb{E}[U^2] < \infty$ . Suppose either of the following conditions is satisfied:

(i)  $\nu$  is an integrable measure on  $\mathbb{R}^{p_z}$ ;

(ii)  $\nu$  is a non-integrable measure on  $\mathbb{R}^{p_z}$  with

$$\int_{\mathbb{R}^{p_z}} 1 \wedge \|s\|^{\alpha} \nu(ds) < \infty, \tag{S.335}$$

and  $\mathbb{E} \|Z\|^{\alpha} < \infty$  for some  $\alpha \in (0, 2)$ ,

then,  $T(U|Z;\nu) = \int_{\mathbb{R}^{p_z}} \left| \mathbb{E}[(U - \mathbb{E}U) \exp(\mathrm{i}Z^{\top}s)] \right|^2 \nu(ds) < \infty.$ 

The above proposition imposes sufficient conditions on  $\nu$  for the resulting metric  $T(U|Z;\nu)$  to be well defined. The first scenario of integrable  $\nu$  corresponds to examples in the literature such as the standard normal density in Antoine and Lavergne (2014, 2022) and Escanciano (2018). The second scenario of a non-integrable  $\nu$  is less explored in the literature. A notable exception is the martingale difference divergence (MDD) metric by Shao and Zhang (2014), which studied a special case using the non-integrable measure of Székely et al. (2007) with  $\nu(ds) = c_{p_z}^{-1} ||s||^{-1-p_z} ds$  for some constant  $c_{p_z} > 0$ , see also Su and Zheng (2017). MDD was later extended by Li et al. (2023) to the generalized martingale difference divergence (GMDD) by allowing for more choices of integrating measures. GMDD serves as the building block of the omnibus tests proposed in this paper. We elaborate further in what follows.

**Proof of Proposition S.3.1**. By the Cauchy-Schwarz inequality, we obtain that

$$\begin{aligned} \left| \mathbb{E}[U \exp(\mathrm{i} Z^{\top} s)] - \mathbb{E}[U] \mathbb{E}[\exp(\mathrm{i} Z^{\top} s)] \right|^2 &\leq \mathrm{Var}(U) \mathbb{E}|\exp(\mathrm{i} Z^{\top} s) - \mathbb{E}\exp(\mathrm{i} Z^{\top} s)|^2 \\ &= \mathrm{Var}(U)(1 - |\mathbb{E}\exp(\mathrm{i} Z^{\top} s)|^2) \end{aligned}$$

This implies that the integrand of  $T(U|Z;\nu)$  is uniformly bounded when  $\mathbb{E}[U^2] < \infty$  since  $|\mathbb{E}\exp(iZ^{\top}s)|^2 \le 1$  by the boundedness of characteristic functions.

(i). This part is trivial since the integrand of  $T(U|Z;\nu)$  is uniformly bounded.

(ii). By (S.335),  $\nu(\{s : ||s|| > 1\})$  is integrable. Hence, it suffices to show the integrability of  $(1 - |\mathbb{E}\exp(iZ^{\top}s)|^2)$  for  $||s|| \le 1$ . Note that for an independent copy  $Z^{\dagger}$  of Z, and  $||s|| \le 1$ , by equation

(2.5) in Davis et al. (2018),

$$1 - |\mathbb{E}[\exp(\mathbf{i}Z^{\top}s)]|^{2} = \int_{\mathbb{R}^{p_{z}}} (1 - \cos(z^{\top}s))\mathbb{P}(Z - Z^{\dagger} \in dz)$$
  
$$\leq \int_{\mathbb{R}^{p_{z}}} (2 \wedge |z^{\top}s|^{2})\mathbb{P}(Z - Z^{\dagger} \in dz)$$
  
$$\leq 2 \int_{|z^{\top}s| \leq \sqrt{2}} |z^{\top}s/\sqrt{2}|^{\alpha}\mathbb{P}(Z - Z^{\dagger} \in dz) + 2\mathbb{P}(|(Z - Z^{\dagger})^{\top}s| > \sqrt{2})$$
  
$$\leq C ||s||^{\alpha}\mathbb{E}||Z - Z^{\dagger}||^{\alpha} < \infty,$$

where C > 0 is some constant, the first inequality holds by the elementary inequality that  $1 - \cos(x) \le 1 \wedge x^2/2$ , and the last inequality holds by the Markov's inequality and the fact that  $|z^{\top}s| \le ||s|| \cdot ||z||$ .

### S.3.2 Characterising the GMDD metric

The following proposition characterizes the class of GMDD metrics.

**Proposition S.3.2.** Let GMDD(U|Z) be a GMDD metric, and denote

$$K(x) = \int_{\mathbb{R}^{p_z}} (1 - \cos(s^{\top} x))\nu(ds).$$
 (S.336)

If  $\mathbb{E}[U^2 + K^2(Z)] < \infty$ , then

$$GMDD(U|Z) = -\mathbb{E}[(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)K(Z - Z^{\dagger})],$$

where  $(U^{\dagger}, Z^{\dagger})$  is an independent copy of (U, Z).

*Proof of Proposition* S.3.2. See proof of Theorem 1 in Li et al. (2023).

In the following, we characterise GMDD metrics via leading examples.

**Example S.3.1** (Integrable  $\nu(\cdot)$  – Fourier Transform). Let  $\nu$  be the probability measure of a random vector  $\xi \in \mathbb{R}^{p_z}$  with symmetric support about the origin. Let  $\phi_{\nu}(\cdot)$  be the Fourier transform of the density

induced by the measure  $\nu$ , i.e.,  $\phi_{\nu}(z) = \int_{\mathbb{R}^{p_z}} \nu(s) \exp(iz^{\top}s) ds$ , then

$$T(U|Z;\nu) = \mathbb{E}[(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)\phi_{\nu}(Z - Z^{\dagger})],$$

see, e.g., Antoine and Lavergne (2014, p. 62). The Fourier transform characterisation leads to ICM metrics based on some commonly used kernel metrics, e.g.,

Gaussian kernel:  $\phi_{\nu}(z) = \exp(-z^{\top}\Sigma z)$ , for some positive definite matrix  $\Sigma$ ;

Laplacian kernel:  $\phi_{\nu}(z) = \exp(-\|z\|/\sigma)$ , for some positive constant  $\sigma$ ; and

Uniform kernel: 
$$\phi_{\nu}(z) = \prod_{l=1}^{p_z} \frac{\sin(a_l z_l)}{a_l z_l}$$
, for  $a_l > 0$ ,  $l = 1, \dots, p_z$ , with the convention  $\frac{\sin(0)}{0} = 1$ 

see, e.g., Gretton et al. (2007).

**Remark S.3.1.** The Fourier transform characterization  $\phi_{\nu}(\cdot)$  in Example S.3.1 suggests two ways of generating integrable kernel metrics:

- 1. setting  $\nu(\cdot)$  to a probability density function which results in a tractable Fourier transform; and
- directly positing a symmetric bounded probability density function (pdf) as φ<sub>ν</sub>(·) whose Fourier transform is strictly positive on ℝ<sup>pz</sup> and non-increasing on (0,∞), see Antoine and Lavergne (2014, p. 62).

While the former involves integration in order to obtain the Fourier transform, the latter is more convenient as one simply chooses appropriate joint probability density functions without deriving Fourier transforms.

**Example S.3.2** (Non-integrable  $\nu(\cdot)$  – Distance). Let  $\nu(s) = c_{p_z}^{-1}(\alpha) ||s||^{-(\alpha+p_z)}$  with  $c_{p_z}(\alpha) = \frac{2\pi^{p_z/2}\Gamma(1-\alpha/2)}{\alpha^{2\alpha}\Gamma((p_z+\alpha)/2)}$ and  $\alpha \in (0,2)$ . This measure is directly adopted from (Székely et al., 2007). It can be shown that

$$T(U|Z;\nu) = -\mathbb{E}[(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)||Z - Z^{\dagger}||^{\alpha}].$$

The leading case,  $\alpha = 1$ , corresponds to the Martingale Difference Divergence (MDD) in Shao and Zhang (2014).

The MDD is scale-invariant and rigid motion invariant with respect to Z, i.e.  $T(U|b + cQZ;\nu) = |c|T(U|Z;\nu)$  for any constants b, c and orthonormal  $Q \in \mathbb{R}^{p_z \times p_z}$ .

**Example S.3.3** (Non-integrable  $\nu(\cdot)$  – Lévy Measure). Let  $\nu(\cdot)$  be a symmetric Lévy measure corresponding to an  $\mathbb{R}^{p_z}$ -valued infinitely divisible random vector  $\xi$  such that (S.335) holds. If  $\xi$  satisfies  $\mathbb{E}||\xi||^{\alpha} < \infty$ , for some  $\alpha \in (0, 2)$ , with characteristic function

$$\vartheta(z) = \exp\Big\{-\int_{\mathbb{R}^{p_z}} [\exp(\mathrm{i} z^\top s) - 1 - \mathrm{i} z^\top s \mathbf{1}(\|s\| \le 1)]\nu(ds)\Big\},\$$

then

$$T(U|Z;\nu) = \operatorname{Re}\mathbb{E}\left[(U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U)\log\vartheta(Z - Z^{\dagger})\right],$$

see Lemma 2.6 in Davis et al. (2018).

**Remark S.3.2.** A special case of Example S.3.3 is obtained by setting  $\xi$  to a sub-Gaussian  $\alpha/2$  stable random vector with characteristic function  $\vartheta(z) = \exp(-|z^{\top}\Sigma z|^{\alpha/2})$  and a positive definite matrix  $\Sigma$ . The resulting metric has the form

$$T(U|Z;\nu) = -\mathbb{E}\left[ (U - \mathbb{E}U)(U^{\dagger} - \mathbb{E}U) | (Z - Z^{\dagger})^{\top} \Sigma (Z - Z^{\dagger}) |^{\alpha/2} \right]$$

With  $\Sigma$  equal to the identity matrix, the ICM metric above coincides with that of Example S.3.2.

The above examples indicate that non-integrable  $\nu(\cdot)$  can be more useful when Z is subject to scaletransformed, rigid-motion-transformed, or when potential violations of (1) occur in the tail of the distribution of Z, i.e., at large values of ||Z||. In the context of ICM specification testing with integrable  $\nu(\cdot)$  for example, large ||Z|| in  $T(U|Z;\nu)$  destroys power, see Bierens (1982, p. 130). Another implication of the above examples is that the integral in (2) can be obtained analytically. This greatly reduces the computational cost due to numerical integration. We tabulate some commonly used kernels in Table S.1.<sup>7</sup>

<sup>&</sup>lt;sup>7</sup>For the Esc6 kernel used in the paper, see Escanciano (2006).

Table S.1: GMDD  $K(\cdot)$  functions

	$ u(\cdot)$	K(z)
Gauss	Standard Normal	$-\exp(-  z  ^2/2)$
MDD	$c_{p_z}^{-1}(1) \ s\ ^{-(1+p_z)}$	z
$\mathrm{SRB}\alpha$	$c_{p_z}^{-1}(\alpha) \ s\ ^{-(\alpha+p_z)}$	$  z  ^{lpha}, \ lpha \in (0,2)$
Laplace	•	$-\exp(-  z  )$
u(Unif)	Uniform [-1,1]	$-\prod_{l=1}^{p_z} \frac{\sin(z_l)}{z_l} \text{ with } \frac{\sin(0)}{0} = 1$
$\nu({\rm Tri})$	Triangular [-1,0,1]	$2\prod_{l=1}^{p_z} \frac{\cos(z_l^2) - 1}{z_l} \text{ with } \frac{\cos(0) - 1}{0} = 1$
Logistic		$-\prod_{l=1}^{p_z}rac{\exp(z_l)}{(1+\exp(z_l))^2}$
Cauchy		$-\prod_{l=1}^{p_{z}}\frac{1}{\pi(1+z_{l}^{2})}$

Notes: The SRB $\alpha$  denotes the Székely et al. (2007) weight with  $\alpha \in (0,2)$ , and MDD is the special case with  $\alpha = 1$ .

## S.4 Relation to CM tests

The proposed test is rooted in ICM tests, but it also shares the advantages of CM tests (Newey, 1985; Tauchen, 1985), which are powerful if prior information on  $\mathbb{H}_a$  is available. For example, if  $\mathbb{E}[U|Z]$ can only take certain types of alternatives  $f_1(Z), \dots, f_{p_f}(Z), p_f \geq 1$ , then setting weight functions in CM tests along the span of these alternatives may yield optimal power (Newey, 1985). Such power enhancement is also allowed in the proposed test by augmenting V with a vector-valued function of Z. In the case of the bivariate  $V = [h(Z), U - h(Z)]^{\top}$  in Lemma 3.1, power enhancement is also achievable by using h(Z) to target alternatives. CM tests, which are closely related to the proposed test, are based on estimates of the form

$$\mathcal{T}_n^{CM} = \sum_{i=1}^n \widetilde{m}(Z_i) U_i,$$

where  $\widetilde{m}(\cdot)$  is a vector of non-degenerate weight functions. Although one may argue that  $m_{\widetilde{V}}(Z) := \mathbb{E}[K(Z-Z^{\dagger})(V^{\dagger}-\mathbb{E}V)|Z]$  in our case plays a role similar to  $\widetilde{m}(Z_i)$  in CM tests, there are fundamental differences.

First, CM tests are not omnibus for any  $\tilde{m}(Z)$  of fixed dimension. There always exist certain forms  $f_1(Z), \dots, f_{p_g}(Z)$  in  $\mu_U(Z)$  under  $\mathbb{H}_a$  such that  $\mathcal{T}_n^{CM}$  has no power; this occurs when U is orthogonal to  $\tilde{m}(Z)$  under  $\mathbb{H}_a$ . This drawback drew much criticism from the literature and may have triggered the rapid development of ICM tests, see, e.g. Bierens (1982, 1990), Bierens and Ploberger (1997), and Delgado et al. (2006). Although the omnibus property for CM tests can be approximately attained by increasing the dimension of  $\tilde{m}(Z_i)$  via non-parametric techniques such as kernel smoothing (which is effectively what non-parametric tests do, e.g., Wooldridge (1992), Yatchew (1992), and Zheng (1996)), our proposed specification test remains omnibus with the dimension of V fixed; the proposed  $\chi^2$ -test can therefore be viewed as a *consistent* CM test.

Second, our specification test allows V to be linearly dependent on U but CM tests do not. This also distinguishes our test from CM tests as GMDD(U|Z) is key to justifying the omnibus property of our test, see the proof of Lemma 3.1. Two independent copies (U, V, Z) and  $(U^{\dagger}, V^{\dagger}, Z^{\dagger})$  are jointly included in  $\delta_V$  while  $\mathbb{E}[\mathcal{T}_n^{CM}] = \mathbb{E}[\tilde{m}(Z)U]$  involves only a single copy. If U is linearly included in the construction of  $\tilde{m}(\cdot)$ , then most likely  $\mathcal{T}_n^{CM}$  is non-null even under  $\mathbb{H}_o$ . A common feature shared by the proposed test and CM tests is the pivotal limiting distribution of the test statistic. This is achieved thanks to the non-degeneracy of  $\tilde{m}(Z)$  and  $m_{\tilde{V}}(Z)$ .

### S.5 Monte Carlo Experiments - Test of Mean Independence

This section examines the empirical size control and power performance of the test of mean independence via simulations. Section S.5.1 presents and discusses five DGPs; Section S.5.2 examines the size control and power performance of the tests of mean independence; Section S.5.3 examines the performance of the  $\chi^2$ -test with V augmented to dimensions  $p_v > 2$ ; Section S.5.4 conducts sensitivity analyses of the size and power performance of the test to variations of the tuning rule  $c_n = \tilde{\lambda}_1 n^{-1/3}$  and other selection criteria used in the literature; Section S.5.5 examines the test of nullity  $\mathbb{E}[U|Z] = \mathbb{E}[U] = 0$  a.s.; and Section S.5.6 compares the running time of the proposed  $\chi^2$ -test with existing ICM-based tests.

#### S.5.1 Specifications

Five different DGPs with conditional heteroskedasticity are considered for the test of mean independence. Each predictor in the set  $\{\xi_1, \xi_2, \iota_1, \iota_2\}$  is standard normally distributed. The predictor set is partitioned into an active set  $\{\xi_1, \xi_2\}$  and an inactive set  $\{\iota_1, \iota_2\}$ . Between partitions, predictors are independent but are correlated within each partition with  $\operatorname{cov}(\xi_1, \xi_2) = \operatorname{cov}(\iota_1, \iota_2) = 0.25$ . Z is set to the inactive set to examine size control. To examine power, Z includes at least one predictor from the active set –  $\gamma$  serves to tune the strength of the deviation from the null under  $\mathbb{H}_a$ . The disturbance  $\mathcal{E}$ is standard normally distributed and independent of all predictors. The following DGPs are considered with  $\gamma \in [0, 1]$ .

MI 1: 
$$U = \xi_1 + \xi_2 + \mathcal{E}/\sqrt{1 + \iota_1^2 + \iota_2^2}, Z = [\iota_1, \iota_2].$$
  
MI 2:  $U = 0.5\gamma\sqrt{\xi_1^2 + \xi_2^2} + \mathcal{E}/\sqrt{1 + \iota_1^2 + \iota_2^2}, Z = [\xi_1, \iota_2].$   
MI 3:  $U = 0.5\gamma I(|\xi_1| < -\Phi^{-1}(1/4)) + \mathcal{E}/\sqrt{1 + \iota_1^2 + \iota_2^2}, Z = [\xi_1, \iota_2].$   
MI 4:  $U = \gamma \frac{\sin(2\xi_1) + \cos(2\xi_2)}{\sqrt{(1 - \exp(-8))/2}} + \mathcal{E}/\sqrt{1 + \iota_1^2 + \iota_2^2}, Z = [\xi_1, \xi_2].$   
MI 5:  $U = 2(\xi_1 + \xi_2)^2/\sqrt{n} + \mathcal{E}/\sqrt{1 + \iota_1^2 + \iota_2^2}, Z = [\xi_1, \xi_2].$ 

One observes from the DGPs above that the mean of U is dependent on the active set but not on the inactive one. DGP MI 1 serves to compare the empirical sizes of tests. The purpose of DGP MI 2 is to examine power against an alternative of non-linear and non-monotone form. DGP MI 3 concerns a binary and non-monotone signal under  $\mathbb{H}_a$  while DGP MI 4 considers a high-frequency alternative. DGP MI 5 serves to examine the power of the tests to detect local alternatives shrinking to zero at the  $\sqrt{n}$  rate. Save MI 1 where U is homoskedastic with respect Z under  $\mathbb{H}_o$ , U is heteroskedastic in all other DGPs. For all DGPs above, the  $\chi^2$ -test is conducted with  $V = [h(Z), U - h(Z)]^{\top}$ ,  $h(Z) = \exp(0.5(Z_1 + Z_2))$ and the regularized inverse is computed using  $c_n = \tilde{\lambda}_1 n^{-1/3}$  where  $\tilde{\lambda}_1$  is the leading eigen-value of  $\tilde{\Omega}_{V,n}$ .

Table S.1: Empirical Size - Test of Mean Independence - DGP MI 1

		10	%			5	76		1%			
n	$\chi^2$	Gauss	MDD	Esc6	$\chi^2$	Gauss	MDD	Esc6	$\chi^2$	Gauss	MDD	Esc6
200	0.093	0.091	0.093	0.094	0.043	0.046	0.048	0.048	0.011	0.006	0.006	0.005
400	0.087	0.097	0.096	0.095	0.042	0.054	0.048	0.044	0.009	0.010	0.007	0.004
600	0.101	0.086	0.083	0.084	0.046	0.047	0.039	0.039	0.011	0.009	0.008	0.009
800	0.091	0.085	0.089	0.091	0.045	0.047	0.043	0.045	0.012	0.011	0.014	0.013

Table S.2: Local Power - DGP MI 5:

		10	%			$5^{\circ}_{2}$	%		1%			
n	$\chi^2$	Gauss	MDD	Esc6	$\chi^2$	Gauss	MDD	Esc6	$\chi^2$	Gauss	MDD	Esc6
200	0.929	0.903	0.712	0.503	0.878	0.849	0.538	0.267	0.721	0.619	0.147	0.054
400	0.939	0.923	0.770	0.551	0.886	0.855	0.598	0.324	0.718	0.644	0.212	0.066
600	0.932	0.939	0.815	0.544	0.886	0.877	0.614	0.337	0.727	0.662	0.225	0.076
800	0.934	0.943	0.814	0.558	0.878	0.879	0.640	0.338	0.724	0.677	0.242	0.077

### S.5.2 Empirical Size and Power

Table S.1 compares the empirical sizes of the proposed  $\chi^2$ -test of mean independence and the bootstrapbased procedures (DGP MI 1) while Table S.2 presents results on local alternatives (DGP MI 5). One observes a good size control and non-trivial local power in Tables S.1 and S.2, respectively, of all tests across all sample sizes and nominal sizes.



Figure S.4: Power Curves - DGP MI 2, n = 400



Figure S.5: Power Curves - DGP MI 3, n=400



Figure S.6: Power Curves - DGP MI 4, n = 400

Figures S.4 to S.6 demonstrate a generally good performance of all tests in detecting deviations from the null. Without incorporating specific information on the direction alternatives may take, the  $\chi^2$ -test of mean independence dominates the bootstrap-based tests in Figures S.4 and S.5 while it is dominated in Figure S.6 by bootstrap-based tests. On the whole, all tests perform reasonably well. That no particular test dominates overall suggests a complementary role played by both the  $\chi^2$ - and bootstrap-based ICM tests of mean independence.

### **S.5.3** $p_v > 2$

The goal of this subsection is to study the sensitivity of the  $\chi^2$ -test to the dimension of V alongside bootstrap-based ICM tests. Consider the following DGP adapted from Section 4.3.

MI 6: 
$$U = \frac{\gamma}{0.233} (\exp(-Z^2/3) - \sqrt{3/5}) + \mathcal{E}, Z \sim \mathcal{N}(0, 1), \text{ and } \mathcal{E} \sim \mathcal{U}[-\sqrt{3}, \sqrt{3}].$$

Define the following:  $h_1(Z) := \exp(Z) - \exp(1/2)$ ;  $h_2(Z) := \sqrt{3} \exp(-Z^2/2) - \sqrt{3/2}$ ;  $V_1 := [h_1(Z), U - h_1(Z), I_2(Z)]^\top$ ;  $V_{1A} := [h_1(Z), U - h_1(Z), h_2(Z)]^\top$ ;  $V_2 := [h_2(Z), U - h_2(Z)]^\top$ ; and  $V_{2A} := [h_2(Z), U - h_2(Z)]^\top$ . Let  $g_p(Z)$  denote a vector of orthogonal polynomials of Z with degrees 1 through p. Then, we generate higher dimensional V given by  $V_{1B}$  and  $V_{2B}$ , respectively, which augment  $V_{1A}$  and  $V_{2A}$  using  $g_2(Z)$ , and  $V_{1C}$  and  $V_{2C}$ , respectively, which augment  $V_{1A}$  and  $V_{2A}$  using  $g_7(Z)$ . When  $p_v \ge 3$ , the

degrees of freedom of the  $\chi^2$ -test is set to the number of positive eigenvalues of  $\widehat{\Omega}_{V,n}$ . In contrast to  $V_2$  where  $h_2(Z)$  targets the alternative,  $V_1$  is agnostic about the alternative.

$\gamma$	Sig-Lev				$\chi^2$ -	test				В	ootstrap	)
_		$V_1$	$V_{1A}$	$V_{1B}$	$V_{1C}$	$V_2$	$V_{2A}$	$V_{2B}$	$V_{2C}$	Gauss	MDD	Esc6
		$p_v = 2$	$p_v = 3$	$p_v = 5$	$p_v = 10$	$p_v = 2$	$p_v = 3$	$p_v = 5$	$p_v = 10$			
	10%	0.088	0.088	0.091	0.093	0.105	0.091	0.094	0.093	0.102	0.101	0.104
0.0	5%	0.039	0.039	0.041	0.042	0.056	0.043	0.047	0.046	0.049	0.051	0.053
	1%	0.006	0.006	0.004	0.004	0.006	0.007	0.006	0.006	0.007	0.009	0.007
-	10%	0.945	0.945	0.943	0.941	0.991	0.973	0.966	0.965	0.927	0.816	0.710
0.2	5%	0.877	0.877	0.873	0.867	0.976	0.937	0.923	0.917	0.852	0.674	0.473
	1%	0.689	0.689	0.655	0.662	0.885	0.810	0.771	0.756	0.614	0.257	0.124
-	10%	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.4	5%	0.997	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.999
	1%	0.979	0.979	0.997	0.993	1.000	1.000	1.000	1.000	1.000	0.998	0.951
-	10%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.6	5	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	1%	0.991	0.991	1.000	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	10%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.8	5%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	1%	0.998	0.998	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
-	10%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
1.0	5%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	1%	0.998	0.998	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table S.3: DGP MI 6 - Sensitivity to  $p_v$ 

Table S.3 presents the power performance of four variations (depending on the dimension and specification of V) of the  $\chi^2$ -test in addition to bootstrap-based tests. First, one observes good size control and non-trivial power increasing in  $\gamma$  of all tests. Second, increasing the dimension of V does not necessarily increase or decrease power. Consider the  $\chi^2$ -tests using  $\{V_1, V_{1A}, V_{1B}, V_{1C}\}$  with  $p_v$  increasing over the set  $\{2, 3, 5, 10\}$  for example. The 5% level test appears to decrease in power at  $\gamma = 0.2$  while it appears to increase in power at  $\gamma = 0.4$ . The effect of  $p_v$  on the power performance in this particular case is therefore inconclusive. A comparison of the test with  $V_2$  (where the alternative is targeted) and  $\{V_1, V_{1A}, V_{1B}, V_{1C}\}$  shows a power advantage of targeting the alternative using a parsimonious 2-dimensional V. Targeting the alternative appears to generate larger power gains than increasing the dimension of V.

### S.5.4 Selection Criteria $c_n$

In all preceding implementations of the proposed  $\chi^2$ -test, the tuning parameter in the regularized  $\widehat{\Omega}_{V,n}$  is set to  $c_n = \widetilde{\lambda}_1 n^{-1/3}$ . This subsection concerns a robustness exercise to examine the sensitivity of the empirical size and power performance to the tuning rule  $c_n$  using DGP MI 6. There are two scenarios to consider.

#### S.5.4.1 Scenario 1

The first scenario concerns sensitivity to the constant  $\iota$  in the rule  $c_n = \tilde{\lambda}_1 n^{-\iota}$ . For the implementation, the set  $\iota \in \{2/5, 1/3, 1/4, 1/6\}$  is considered with  $p_v = 2$ , and  $V = V_1$  from Section S.5.3.

Table S.4 presents results that compare the performance of the  $\chi^2$ -test by different choices of  $c_n$  in the first scenario. A clear conclusion is that the results are robust to the choice of  $\iota$  in the rule  $c_n = \tilde{\lambda}_1 n^{-\iota}$  as there are negligible numerical differences in the empirical size and power across different valid choices of  $\iota \in (0, 1/2)$ .

#### S.5.4.2 Scenario 2

The second scenario compares the  $\chi^2$ -test with, in addition to  $c_n$  in Scenario 1 above, suitable selection criteria typically used for truncated singular value decomposition – see Falini (2022) for a review. The setting adopted in this scenario is DGP MI 6,  $p_v = 10$ , and  $V = V_{1C}$  from Section S.5.3. From Section 4.2, recall  $p(c_n)$  is the number of non-zero eigenvalues in the regularized  $\widehat{\Omega}_{V,n}$ . Define

$$E_l := -\frac{1}{\log(p_v)} \sum_{l'=1}^l \widetilde{f}_{l'} \log(\widetilde{f}_{l'}) \text{ where } \widetilde{f}_l := \widetilde{\lambda}_l^2 / \sum_{l'=1}^{p_v} \widetilde{\lambda}_{l'}^2.$$

The following suitable SVD selection criteria are defined in terms of  $p(c_n)$ .

$\gamma$	Sig-Lev		$c_n = \hat{\lambda}$	$\tilde{\lambda}_1 n^{-\iota}$	
		$\iota = \frac{2}{5}$	$\iota = \frac{1}{3}$	$\iota = \frac{1}{4}$	$\iota = \frac{1}{6}$
	10%	0.087	0.085	0.085	0.085
0.0	5%	0.044	0.042	0.042	0.042
	1%	0.009	0.009	0.009	0.009
	10%	0.303	0.303	0.302	0.302
0.2	5%	0.189	0.189	0.188	0.188
	1%	0.049	0.049	0.048	0.048
	10%	0.757	0.757	0.757	0.757
0.4	5%	0.632	0.632	0.632	0.632
	1%	0.315	0.315	0.314	0.314
	10%	0.937	0.937	0.937	0.937
0.6	5%	0.871	0.871	0.871	0.871
	1%	0.665	0.665	0.665	0.665
	10%	0.980	0.980	0.980	0.980
0.8	5%	0.958	0.958	0.958	0.958
	1%	0.835	0.835	0.835	0.835
	10%	0.989	0.989	0.989	0.989
1.0	5%	0.980	0.980	0.980	0.980
	1%	0.922	0.920	0.920	0.920

Table S.4: DGP MI 6 - Sensitivity to  $\iota$ 

- (1) R-B ratio-based selection;  $p(c_n) = \underset{1 \le l \le p_v}{\operatorname{arg\,min}} \frac{\lambda_{l+1}}{\lambda_l}$ ; references: Lam et al. (2011), Lam and Yao (2012), and Lee and Shao (2018, eqn. 6).
- (2)  $E\iota$  entropy-based selection;  $p(c_n) = \min\left\{1 \le l \le p_v : E_l \ge \iota E_{p_v}\right\}$ ; references: Alter et al. (2000) and Falini (2022, Sect. 2.6).
- (3) TV $\iota$  Total Variance based selection;  $p(c_n) = \sum_{l=1}^{p_v} \mathbb{1}\{\widetilde{f}_l \ge \iota\}$ ; references: Suhr (2005) and Falini (2022, Sect. 2.6).
- (4) CTV $\iota$  Cumulative percentage of Total Variance based selection;  $p(c_n) = \min \left\{ 1 \leq l \leq p_v : \sum_{l'=1}^{l} \widetilde{f}_{l'} \geq \iota \right\}$ ; references: Jolliffe (2002, Chapter 6) and Falini (2022, Sect. 2.6).

Recall  $\widetilde{\Omega}_{V,n}$  is positive semi-definite hence the  $\widetilde{f}_l$ ,  $l = 1, \ldots, p_v$  are in descending order given a descending ordering of the eigenvalues  $\widetilde{\lambda}_l$ ,  $l = 1, \ldots, p_v$ . This ensures that  $p(c_n)$  per any of the above selection criteria corresponds to the largest  $p(c_n)$  eigenvalues and the corresponding  $c_n$  is implicitly defined.

Table S.5 compares the size control and power performance of the  $\chi^2$ -test with different choices of the regularization parameter  $c_n$ . Besides the ratio-based estimator which fails to deliver a  $\chi^2$ -test that controls size, the other choices lead to meaningful size control. One observes non-trivial power under  $\mathbb{H}_a$ . This exercise and that of Scenario 1 confirm the reliability and robustness of the selection rule  $c_n = \tilde{\lambda}_1 n^{-1/3}$  used in this paper.

### S.5.5 Test of Nullity

 $\mathbb{H}_{o}^{*}$ :  $\mathbb{E}[U|Z] = \mathbb{E}[U] = 0$  a.s. is violated if either  $\mathbb{E}[U] \neq 0$  or  $\mathbb{E}[U|Z] \neq \mathbb{E}[U]$  a.s. To compare the performance of the  $\chi^{2}$ -test of the hypothesis of nullity  $\mathbb{H}_{o}^{*}$ , we take the following modified versions of DGP MI 6.

MI 6':  $U = \frac{\gamma}{0.233}\sqrt{3/5} + \mathcal{E}, Z \sim \mathcal{N}(0, 1) \text{ and } \mathcal{E} \sim \mathcal{U}[-\sqrt{3}, \sqrt{3}].$ MI 6'':  $U = \frac{\gamma}{0.233} \exp(-Z^2/3) + \mathcal{E}, Z \sim \mathcal{N}(0, 1) \text{ and } \mathcal{E} \sim \mathcal{U}[-\sqrt{3}, \sqrt{3}].$ 

			$(c_n =$	$\widetilde{\lambda}_1 n^{-\iota}$				Sel	lection C	riteria		
$\gamma$	Sig-Lev	$\iota = \frac{2}{5}$	$\iota = \frac{1}{3}$	$\iota = \frac{1}{4}$	$\iota = \frac{1}{6}$	R-B	E.7	E.9	TV.05	TV.10	CTV.7	CTV.9
	10%	0.090	0.093	0.092	0.088	0.376	0.093	0.089	0.093	0.091	0.084	0.090
0.0	5%	0.042	0.042	0.042	0.041	0.363	0.042	0.041	0.042	0.040	0.044	0.039
	1%	0.004	0.004	0.004	0.005	0.343	0.004	0.004	0.004	0.005	0.008	0.005
	10%	0.928	0.941	0.937	0.632	0.824	0.943	0.906	0.933	0.724	0.291	0.752
0.2	5%	0.853	0.867	0.864	0.538	0.765	0.872	0.833	0.861	0.637	0.188	0.664
	1%	0.650	0.662	0.657	0.347	0.630	0.665	0.628	0.654	0.437	0.073	0.462
	10%	1.000	1.000	1.000	0.939	1.000	1.000	1.000	1.000	0.967	0.718	0.982
0.4	5%	1.000	1.000	0.999	0.897	1.000	1.000	1.000	0.999	0.940	0.615	0.965
	1%	0.984	0.993	0.993	0.786	0.999	0.996	0.981	0.991	0.858	0.384	0.905
	10%	1.000	1.000	1.000	0.997	1.000	1.000	1.000	1.000	0.999	0.928	1.000
0.6	5%	1.000	1.000	1.000	0.990	1.000	1.000	1.000	1.000	0.998	0.877	1.000
	1%	0.999	0.999	0.999	0.946	1.000	1.000	0.999	0.999	0.971	0.729	0.989
	10%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.990	1.000
0.8	5%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.973	1.000
	1%	1.000	1.000	1.000	0.992	1.000	1.000	1.000	1.000	0.996	0.903	0.999
	10%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.997	1.000
1.0	5%	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.995	1.000
	1%	1.000	1.000	1.000	0.994	1.000	1.000	1.000	0.999	0.997	0.964	0.999

Table S.5: DGP MI 6 - SVD selection criteria

Notes: The first four columns use the regularization technique used in this paper with  $c_n = \tilde{\lambda}_1 n^{-\iota}$ ,  $\iota \in \{2/5, 1/3, 1/4, 1/6\}$ , respectively. R-B is the ratio-based selection criterion,  $E_{\ell}$ ,  $\iota \in \{.7, .9\}$  is the  $\alpha$  fraction of total entropy selection criterion,  $TV_{\ell}$ ,  $\iota \in \{.05, .10\}$  is the  $\alpha$  of total variance selection criterion,  $CTV_{\ell}$ ,  $\iota \in \{.7, .9\}$  is the cumulative percentage of the total variance selection criterion.

										~	
		DGF	• MI 6′,	$c_n = \lambda_1$	$n^{-\iota}$			DGP	• MI 6",	$c_n = \lambda_1$	$n^{-\iota}$
$\gamma$	Sig-Lev	$\iota = \frac{2}{5}$	$\iota = \frac{1}{3}$	$\iota = \frac{1}{4}$	$\iota = \frac{1}{6}$	$\gamma$	Sig-Lev	$\iota = \frac{2}{5}$	$\iota = \frac{1}{3}$	$\iota = \frac{1}{4}$	$\iota = \frac{1}{6}$
	10%	0.087	0.085	0.085	0.085		10%	0.087	0.085	0.085	0.085
0.0	5%	0.044	0.042	0.042	0.042	0.0	5%	0.044	0.042	0.042	0.042
	1%	0.009	0.009	0.009	0.009		1%	0.009	0.009	0.009	0.009
	10%	0.999	0.986	0.977	0.977		10%	0.941	0.822	0.817	0.817
0.2	5%	0.997	0.969	0.948	0.948	0.2	5%	0.885	0.683	0.678	0.678
	1%	0.991	0.873	0.807	0.807		1%	0.774	0.410	0.400	0.400
	10%	1.000	1.000	1.000	1.000		10%	1.000	1.000	1.000	1.000
0.4	5%	1.000	1.000	1.000	1.000	0.4	5%	1.000	1.000	1.000	1.000
	1%	1.000	1.000	1.000	1.000		1%	1.000	1.000	1.000	1.000
	10%	1.000	1.000	1.000	1.000		10%	1.000	1.000	1.000	1.000
0.6	5%	1.000	1.000	1.000	1.000	0.6	5%	1.000	1.000	1.000	1.000
	1%	1.000	1.000	1.000	1.000		1%	1.000	1.000	1.000	1.000
	10%	1.000	1.000	1.000	1.000		10%	1.000	1.000	1.000	1.000
0.8	5%	1.000	1.000	1.000	1.000	0.8	5%	1.000	1.000	1.000	1.000
	1%	1.000	1.000	1.000	1.000		1%	1.000	1.000	1.000	1.000
_	10%	1.000	1.000	1.000	1.000		10%	1.000	1.000	1.000	1.000
1.0	5%	1.000	1.000	1.000	1.000	1.0	5%	1.000	1.000	1.000	1.000
	1%	1.000	1.000	1.000	1.000		1%	1.000	1.000	1.000	1.000

Table S.6: DGPs MI  $6^\prime$  and MI  $6^{\prime\prime}$ 

 $\gamma \neq 0$  corresponds to  $\mathbb{E}[U] \neq 0$  in MI 6' and to  $\mathbb{E}[U|Z] \neq \mathbb{E}[U]$  a.s. in DGP MI 6".

Table S.6 presents results on DGPs MI 6' and MI 6'' using the framework of Table S.4 but with a focus on the power performance under either violation of  $\mathbb{H}_o^*$ . From both sets of columns corresponding to DGPs MI 6' and MI 6'', one observes from Table S.6 that the  $\chi^2$ -test of nullity has good size control and non-trivial power under both violations:  $\mathbb{E}[U] = 0$  and  $\mathbb{E}[U|Z] = \mathbb{E}[U]$  a.s.

### S.5.6 Running Time

An advantage of pivotalizing the ICM test of mean independence is the gain in computational time. The computational advantage in addition to the pivotality of the test can be very useful in tasks such as feature screening in (ultra-) high dimensions, see e.g., Shao and Zhang (2014). The following exercise serves to give an idea of the computational gain relative to bootstrap-based procedures.

	Average Running Time (seconds)				Median Relative Time		
n	$\chi^2$	Gauss	MDD	Esc6	Gauss	MDD	Esc6
200	0.004	0.047	0.048	0.202	13.333	13.333	57.667
	(0.001)	(0.080)	(0.019)	(0.031)	(4.500)	(4.917)	(23.667)
400	0.010	0.157	0.153	1.458	17.056	16.778	160.111
	(0.002)	(0.008)	(0.007)	(0.035)	(5.542)	(5.933)	(59.479)
600	0.020	0.354	0.349	4.660	19.243	19.111	257.722
	(0.004)	(0.011)	(0.009)	(0.048)	(5.512)	(5.853)	(82.725)
800	0.035	0.692	0.689	10.845	21.365	21.594	338.937
	(0.006)	(0.019)	(0.016)	(0.049)	(5.638)	(6.426)	(103.268)

Table S.7: Running Time - Test of Mean Independence - DGP MI 1

Notes: The second row (in parentheses) for each sample size includes standard deviations and inter-quartile ranges for the average running times and relative times (with the  $\chi^2$ -test as the benchmark), respectively.

Table S.7 compares the running time of tests. One observes from Table S.7 that the proposed  $\chi^2$ -test of mean independence on average incurs a negligible computational cost, unlike the bootstrap-based procedures that incur substantial computational costs at large sample sizes. This observation is also borne out by the relative computational times. Across all sample sizes, the relative computational times indicate a considerable computational gain from using the proposed  $\chi^2$ -test of mean independence.

### S.6 Numerical Computation of the Bahadur lopes

This section outlines details pertaining to the Monte Carlo numerical integration used to obtain the Bahadur slopes in Section 4.3. The approach proceeds by computing  $\mathbb{E}[a(Z)a(Z^{\dagger})K(Z-Z^{\dagger})]$ ,  $\lambda_1$ ,  $a_o$ , and  $\Omega_{V_a}$  on a sample of 1 000 random draws following the DGP in Section 4.3.  $\lambda_1 = 0.6175762$  is computed using steps 1-3 of Seri (2022, Algorithm 1) with (i, j)'th element  $\exp(-0.5(Z_i - Z_j)^2)\mathcal{E}_i\mathcal{E}_j/(n-1)$ . The numerical values of the Bahadur slopes in Table 4.1 are then obtained using averages of the quantities  $\mathbb{E}[a(Z)a(Z^{\dagger})K(Z-Z^{\dagger})]$ ,  $\lambda_1$ ,  $a_o$ , and  $\Omega_{V_a}$  over 10 000 replications.

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