Kernel Conditional Moment Test via Maximum Moment Restriction

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Abstract

We propose a new family of specification tests called kernel conditional moment (KCM) tests. Our tests are built on conditional moment embeddings (CMME)—a novel representation of conditional moment restrictions in a reproducing kernel Hilbert space (RKHS). After transforming the conditional moment restrictions into a continuum of unconditional counterparts, the test statistic is defined as the maximum moment restriction within the unit ball of the RKHS. We show that the CMME fully characterizes the original conditional moment restrictions, leading to consistency in both hypothesis testing and parameter estimation. The proposed test also has an analytic expression that is easy to compute as well as closed-form asymptotic distributions. Our empirical studies show that the KCM test has a promising finite-sample performance compared to existing tests.

Keywords — conditional moment restriction, kernel mean embedding, reproducing kernel Hilbert space, generalized method of moments.

1 Introduction

Many problems in causal inference, economics, and finance are often formulated as a conditional moment restriction (CMR): for correctly specified models, the conditional mean of certain functions of data is almost surely equal to zero (Newey 1993). Rational expectation models—widely used in many fields of macroeconomics—specify how economic agents exploit available information to form their expectations in terms of conditional moments (Muth 1961). Recent advances in causal machine learning also rely on the CMR including a generalized random forest (GRF)
Figure 1: **Conditional moment embedding (CMME):** The conditional moments $E[\psi(Z; \theta)|X]$ for different parameters $\theta$ are uniquely ($P_X$-almost surely) embedded into the RKHS. The RKHS norm of $\mu_\theta$ measures to what extent these restrictions are violated and hence is used as a test statistic for conditional moment tests.

(Atthey et al. 2019), orthogonal random forest (ORF) (Oprescu et al. 2019), double machine learning (DML) (Chernozhukov et al. 2018), and nonparametric instrumental variable regression (Bennett et al. 2019, Lewis and Syrgkanis 2018) among others; see also Hartford et al. (2017), Singh et al. (2019), Muandet et al. (2019) and references therein.

Checking the validity of these moment restrictions is the first and foremost step to ensure that a model is correctly specified which constitutes a fundamental assumption for its estimation and inference. A model misspecification often creates biases to parameter estimates, inconsistency of standard errors, and invalid asymptotic distributions that hinder our subsequent inference based on the model. An overidentifying restriction test in the generalized method of moments (GMM) framework is one of the standard approaches to test a finite number of unconditional moment conditions (Hansen 1982, Hall 2005). The $J$-test is an example of such tests (Sargan 1958, Hansen 1982), and a variety of tests have been developed in econometrics to deal with various sources of misspecification; see, e.g., Bierens (2017) for a review. In this paper, we focus on an important class of CMR-based specification tests known as the conditional moment (CM) tests (Newey 1985, Tauchen 1985) which have a long history in econometrics (Hausman 1978, White 1981, Newey 1993, Bierens 2017).

Testing **conditional** moment restrictions becomes more challenging as an **infinite** number of equivalent unconditional moment restrictions (UMR) must be examined simultaneously (cf. Section 3). At first, Newey (1985) and Tauchen (1985) proposed to perform the overidentifying restriction test on a **finite** subset of the UMR. Unfortunately, the CM tests that rely only on a finite number of moment conditions cannot be consistent against all alternatives. Additional assumptions such as the global identification of selected moment conditions and sample-size dependent moment conditions are required to guarantee consistency (de Jong 1996, Donald et al. 2003). To overcome this limitation, Bierens (1982) introduced the first consistent CM tests—known as integrated conditional moment (ICM) tests—by checking all moment conditions simultaneously (Bierens and Ploberger 1997). However, the
ICM test depends on parametric weighting functions and nuisance parameters that limit its practical use. An alternative class of consistent CM tests, known as smooth tests, employ nonparametric kernel estimation\(^1\) (Zheng 1996, Li and Wang 1998) which also forms a basis for the generalized empirical likelihood (GEL) approach (Delgado et al. 2006, Tripathi and Kitamura 2003). However, they have non-trivial power only against local alternatives that approach the null at a slower rate than \(1/\sqrt{n}\), and are susceptible to the curse of dimensionality (cf. Section 5 for the discussion).

Inspired by a surge of kernel-based tests (Gretton et al. 2012, Chwialkowski et al. 2016, Liu et al. 2016), we propose to embed the CMR in a reproducing kernel Hilbert space (RKHS). This allows us to develop a class of consistent CM tests that we call kernel conditional moment (KCM) tests (cf. Section 4). By transforming CMR into a continuum of UMR in RKHS, the test statistic is defined as the maximum moment restriction (MMR) within the unit ball of the RKHS (cf. Section 3). We show that the MMR corresponds to the RKHS norm of Hilbert space embedding of conditional moments which uniquely determine the original CMR (cf. Theorem 3.2). Moreover, while allowing us to incorporate an infinite number of moment conditions, the MMR has a closed-form expression which makes it easy to use in practice (cf. Theorem 3.3 and 3.4). Our framework also has relationships to existing methods in econometrics and machine learning (cf. Section 5). To the best of our knowledge, the use of reproducing kernels to model conditional moment restrictions has never appeared elsewhere in the literature.

All proofs can be found in Appendix C.

2 Background

We introduce the CMR in Section 2.1 and then review the concepts of kernels and RKHS in Section 2.2. Finally, we discuss the main assumptions in Section 2.3.

2.1 Conditional Moment Restrictions

Let \(Z\) be a random variable taking values in \(Z \subseteq \mathbb{R}^p\) with distribution \(P_Z\), \(X\) a subvector of \(Z\) taking values in \(X \subseteq \mathbb{R}^d\) with distribution \(P_X\), and \(\Theta \subset \mathbb{R}^r\) a parameter space. Following Newey (1993), we consider models where the only available information about the unknown parameter \(\theta_0 \in \Theta\) is a set of conditional moment restrictions

\[
\mathcal{M}(X; \theta_0) := E[\psi(Z; \theta_0)|X] = 0, \quad P_X-\text{a.s.,}
\]

where \(\psi : Z \times \Theta \to \mathbb{R}^q\) is a vector of generalized residual functions whose functional forms are known up to the parameter \(\theta \in \Theta\). The expectation is always taken over all random variables that are not conditioned on. We denote by \(\theta_0\) an ideal parameter that satisfies (1). Note that there can be two different models that are observationally equivalent on the basis of (1) alone.

Several statistical problems can be formulated as (1). In nonparametric regression models, \(Z = (X, Y)\) where \(Y \in \mathbb{R}\) is a dependent variable and \(\psi(Z; \theta) = Y - f(X; \theta)\). For conditional quantile models, \(Z = (X, Y)\) and \(\psi(Z; \theta) = 1\{Y < \}

\(^1\)The smooth tests employ a kernel density estimator (KDE), which differs fundamentally from the notion of reproducing kernels considered in this work (cf. Section 5).
\( f(X; \theta) \) is estimated using this data and hence the test performance is also subject to the estimation error. A generalization of our framework to those cases will require more involved analyses, and we leave it to future work.

### 2.2 Reproducing Kernel Hilbert Spaces

Let \( \mathcal{X} \) be a non-empty set and \( \mathcal{F} \) a Hilbert space consisting of functions on \( \mathcal{X} \) with \( \langle \cdot, \cdot \rangle_\mathcal{F} \) and \( \| \cdot \|_\mathcal{F} \) being its inner product and norm, respectively. The Hilbert space \( \mathcal{F} \) is called a reproducing kernel Hilbert space (RKHS) if there exists a symmetric function \( k : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) called the reproducing kernel of \( \mathcal{F} \) such that (i) \( k(x, \cdot) \in \mathcal{F} \) for all \( x \in \mathcal{X} \) and (ii) \( f(x) = \langle f, k(x, \cdot) \rangle_\mathcal{F} \) for all \( f \in \mathcal{F} \) and \( x \in \mathcal{X} \). The latter is called the reproducing property of \( \mathcal{F} \). Every positive definite kernel \( k \) uniquely determines the RKHS for which \( k \) is a reproducing kernel (Aronszajn 1950).

Let \( \{ (\lambda_j, e_j) \} \) be pairs of positive eigenvalues and orthonormal eigenfunctions of \( k \), i.e., \( \int e_i(x)e_j(x) \, dx = 1 \) if \( i = j \) and zero otherwise. By Mercer’s theorem (Steinwart and Christmann 2008; Thm 4.49), the kernel \( k \) has the spectral decomposition

\[
   k(x, x') = \sum_j \lambda_j e_j(x)e_j(x'), \quad x, x' \in \mathcal{X},
\]

where the convergence is absolute and uniform. As a result, for any \( f \in \mathcal{F} \), we have \( f(x) = \sum_j f_j e_j(x) \) with \( \sum_j f_j^2 / \lambda_j < \infty \) where \( f_j = \langle f, e_j \rangle_\mathcal{F}, \langle f, g \rangle_\mathcal{F} = \sum_j f_j g_j / \lambda_j \), and \( \| f \|_\mathcal{F}^2 = \langle f, f \rangle_\mathcal{F} = \sum_j f_j^2 / \lambda_j \).

Next, we introduce the notion of integrally strictly positive definite (IPD) kernels and Bochner’s characterization.

**Definition 2.1.** (IPD). A kernel \( k(x, x') \) is integrally strictly positive definite (IPD) if for any function \( f \) that satisfies \( 0 < \| f \|_\mathcal{F}^2 < \infty \),

\[
   \int_{\mathcal{X}} f(x)k(x, x')f(x') \, dx \, dx' > 0.
\]
The IPD kernel is an important notion in kernel methods and is closely related to characteristic and universal kernels, see, e.g., Simon-Gabriel and Schölkopf (2018).

**Theorem 2.1** (Bochner). A continuous function $\varphi : \mathbb{R}^d \to \mathbb{C}$ is positive definite if and only if it is the Fourier transform of a finite nonnegative Borel measure $\Lambda$ on $\mathbb{R}^d$, i.e.,

$$
\varphi(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ix^\top \omega} d\Lambda(\omega)
$$

for $x \in \mathbb{R}^d$.

Examples of popular kernels are the Gaussian RBF kernel $k(x, x') = \exp(-\|x - x'\|_2^2 / 2\sigma^2), \sigma > 0$, Laplacian kernel $k(x, x') = \exp(-\|x - x'\|_1 / \sigma), \sigma > 0$, and inverse multiquadric (IMQ) kernel $k(x, x') = (c^2 + \|x - x'\|_2^2)^{-\gamma}, c, \gamma > 0$. See, e.g., Steinwart and Christmann (2008; Ch. 4) and Schölkopf and Smola (2002) for more details.

### 2.3 Main Assumptions

Our subsequent analyses rely on these key assumptions.

(A1) The random vector $(X, Z)$ forms a strictly stationary process with the probability measure $P_{XZ}$.

(A2) Regularity conditions: (i) the function $\psi : Z \times \Theta \to \mathbb{R}^q$ where $q < \infty$ is continuous on $\Theta$ for each $z \in Z$; (ii) $E[\psi(Z; \theta)|x]$ exists and is finite for every $\theta \in \Theta$ and $x \in X$ for which $P_X(x) > 0$; (iii) $E[\psi(Z; \theta)|x]$ is continuous on $\Theta$ for all $x \in X$ for which $P_X(x) > 0$.

(A3) Global identification: there exists a unique $\theta_0 \in \Theta$ for which $E[\psi(Z; \theta_0)|X] = 0$ a.s., and $P(E[\psi(Z; \theta)|X] = 0) < 1$ for all $\theta \in \Theta, \theta \neq \theta_0$.

(A4) The kernel $k$ is IPD, continuous, and bounded, i.e., $\sup_{x \in X} \sqrt{k(x, x)} < \infty$.

Assumption (A1) ensures that all expectations of functions of $(X, Z)$ are independent of time. The regularity conditions (A2) are standard assumptions (Hall 2005; Ch. 3) which ensure that $\psi$ is well-defined, and hold in most models considered in the literature (Hall 2005). By contrast, (A3) may not hold, especially in non-linear models. One can assume local identification instead, but this requires further restrictions on $\psi$. Lastly, (A4) implies that the RKHS $\mathcal{F}$ consists of bounded continuous functions (Steinwart and Christmann 2008; Sec. 4.3) and is expressive enough (cf. Theorem 3.2).

### 3 Maximum Moment Restriction

In this section, we present the RKHS representation of the CMR in (1). Let $\mathcal{F}$ be a set of measurable functions on $X$. Then, by the law of iterated expectation,

$$
E_{XZ}[\psi(Z; \theta)f(X)] = E_X[E_Z[\psi(Z; \theta)f(X)|X]] = E_X[E_{XZ}[\mathcal{M}(X; \theta)f(X)]]
$$

for any $f \in \mathcal{F}$. That is, the CMR in (1) implies an infinite set of unconditional moment restrictions

$$
E[\psi(Z; \theta_0)f(X)] = 0, \quad \forall f \in \mathcal{F},
$$

(4)
Equivalently, any \( \theta_0 \in \Theta \) that satisfies (4) must also satisfy what we call a maximum moment restriction (MMR)

\[
\sup_{f \in \mathcal{F}} \| E[\psi(Z; \theta_0) f(X)] \|_2^2 = 0.
\]  

(5)

It is well known that the parameters of interest need not be globally identified by the implied moment restrictions (4) and (5). We call \( \mathcal{F} \) for which (5) implies (1) a sufficient class of instruments. For the CM test to be consistent against all alternatives, \( \mathcal{F} \) must consist of infinitely many instruments. However, when \( \mathcal{F} \) is infinite, the sup operator makes it hard to optimize (5). We resolve these issues by choosing \( \mathcal{F} \) to be a unit ball in an RKHS, which we show to be a sufficient class of instruments. As a result, (5) can be solved analytically, the parameters of interest can be consistently estimated, and the resulting CM test is consistent against all fixed alternatives.

Lewis and Syrgkanis (2018) and Bennett et al. (2019) recently propose to estimate \( \theta_0 \) based on (5) and \( \mathcal{F} \) that is parameterized by deep neural networks. While they consider an estimation problem, we focus on hypothesis testing problems. Nevertheless, our formulation of CMR can also be used to estimate \( \theta_0 \) (cf. Section 3.2 and Appendix B). Note that the algorithms proposed in Lewis and Syrgkanis (2018), Bennett et al. (2019) require solving a minimax game, whereas our approach for estimation is simply a minimization problem.

3.1 Conditional Moment Embedding

To express (5) using the RKHS, we first develop a new representation of the CMR in a vector-valued RKHS of functions \( f : \mathcal{X} \rightarrow \mathbb{R}^q \) (Álvarez et al. 2012). Let \( \mathcal{F} \) be the RKHS of real-valued functions on \( \mathcal{X} \) with reproducing kernel \( k \) and \( \mathcal{F}^q \) the product RKHS of functions \( f := (f_1, \ldots, f_q) \) where \( f_i \in \mathcal{F} \) for all \( i \) with an inner product \( \langle f, g \rangle_{\mathcal{F}^q} = \sum_{i=1}^q \langle f_i, g_i \rangle_{\mathcal{F}} \) and norm \( \| f \|_{\mathcal{F}^q} = \sqrt{\sum_{i=1}^q \| f_i \|_{\mathcal{F}}^2} \). For \( \theta \in \Theta \), we define a conditional moment operator \( M_\theta \) on \( \mathcal{F}^q \) as

\[
M_\theta f := E[\psi(Z; \theta)^\top f(X)] = \sum_{i=1}^q E[\psi_i(Z; \theta) f_i(X)],
\]

where \( \psi_i \) denotes the \( i \)-th component of \( \psi \). This operator takes an instrument \( f \in \mathcal{F}^q \) as input and returns the corresponding conditional moment restrictions.

The following lemma shows that \( M_\theta \) satisfies the property of the original conditional moment restrictions.

**Lemma 3.1.** For all \( f \in \mathcal{F}^q \), \( M_\theta f = 0 \).

Moreover, it is not difficult to see that

\[
|M_\theta f| \leq \sum_{i=1}^q \| f_i \|_{\mathcal{F}} \sqrt{E[\psi_i(Z; \theta) \psi_i(Z'; \theta) k(X, X')] < \infty
\]

where \( (X', Z') \) is an independent copy of \( (X, Z) \). Hence, \( M_\theta \) is a bounded linear operator. By Riesz’s representation theorem (Kreyszig 1989; Ch. 3.8), there exists
a unique element $\mu_θ$ in $F_q$ such that $M_θ f = \langle f, \mu_θ \rangle_{F_q}$ for all $f \in F_q$. Indeed, by the reproducing property,

$$M_θ f = \sum_{i=1}^q \langle f, E[ξ_i(X,Z)] \rangle_{F_q} = \langle f, E[ξ_i(X,Z)] \rangle_{F_q},$$

where $ξ_θ(x,z) := (ψ_1(z;θ)k(x,·),...,ψ_q(z;θ)k(x,·))$ is the feature map in $F_q$ and $ξ_θ$ denotes the $i$-th element of $ξ_θ$. The above equalities are well-defined since $ξ_θ(x,z)$ is Bochner integrable (Steinwart and Christmann 2008; Def. A.5.20), i.e., $E\|ξ_θ(X,Z)\|_{F_q} \leq \sqrt{E\|ξ_θ(X,Z)\|^2_{F_q}} = \sqrt{E[ψ(Z;θ)\cdot ψ(Z;θ)k(X,X)]} < \infty$. In other words, $\mu_θ := E[ξ_θ(X,Z)]$ is a representer of $M_θ$ in $F_q$. We define $\mu_θ$ as a conditional moment embedding (CMME) of $E[ψ(Z;θ)|X]$ in $F_q$ relative to $P_X$.

**Definition 3.1.** For each $θ \in Θ$, let $ξ_θ(x,z) := (ψ_1(z;θ)k(x,·),...,ψ_q(z;θ)k(x,·)) \in F_q$. The conditional moment embedding (CMME) is defined as

$$\mu_θ := E_{XZ}[ξ_θ(X,Z)] \in F_q.$$

The CMME $\mu_θ$ in (6) takes the form of a kernel mean embedding of $P_{XZ}$ with the feature map $ξ_θ$ (Smola et al. 2007, Berlinet and Thomas-Agnan 2004, Muandet et al. 2017) as illustrated in Figure 1. Hence, given an i.i.d. sample $(x_i,z_i)_{i=1}^n$ from $P_{XZ}$, we can estimate $\mu_θ$ by $\tilde{μ}_θ := \frac{1}{n} \sum_{i=1}^n ξ_θ(x_i,z_i)$. The following theorem establishes the $\sqrt{n}$-consistency of this estimator.

**Theorem 3.1.** Assume that $\|ξ_θ(X,Z)\|_{F_q} < C_θ < \infty$ almost surely for a fixed constant $C_θ$. Let $σ_θ^2 := E\|ξ_θ(X,Z)\|^2_{F_q}$. Then, for any $θ \in Θ$ and $0 < δ < 1$, with probability at least $1 - δ$,

$$\|\tilde{μ}_θ - μ_θ\|_{F_q} \leq \frac{2C_θ \log \frac{4}{δ}}{n} + \sqrt{\frac{2σ_θ^2 \log \frac{4}{δ}}{n}} \ .
$$

Remarkably, $\tilde{μ}_θ$ converges at a rate $O_p(n^{-1/2})$ that is independent of the dimension of $(X,Z)$ and that of the RKHS $F_q$. This is an appealing property as estimation and inference based on $\tilde{μ}_θ$ become less susceptible to the curse of dimensionality (see, e.g., Khoasravi et al. (2019) and references therein for the discussion). Under certain assumptions, Tolstikhin et al. (2017) established the minimax optimal rate for the kernel mean estimators like $\tilde{μ}_θ$.

The next theorem shows that $μ_θ$ provides a unique representation of the CMR $ℳ(X,θ)$ in $F_q$ relative to $P_X$.

**Theorem 3.2.** If the kernel $k$ is IPD, then for any $θ_1,θ_2 \in Θ$, $ℳ(x;θ_1) = ℳ(x;θ_2)$ for $P_X$-almost all $x$, i.e., $B_θ := \{ x \in X : ℳ(x;θ_1) = ℳ(x;θ_2) = 0 \} \Rightarrow P_X(B_θ) = 1$, if and only if $μ_θ_1 = μ_θ_2$.

To better understand Theorem 3.2, consider when $q = 1$ and $k(x,x') = ϕ(x-x')$ is a shift-invariant kernel. First, we have $μ_θ(·) = E_X[ξ_θ(Z;θ)k(X,·)|X] = E_X[E_Z[ψ(Z;θ)|X]|k(X,·)] = E_X[ℳ(X;θ)k(X,·)]$. It is then easy to show using Theorem 2.1 that

$$μ_θ(·) = \int_{R^d} \phi(ω;θ)c(ω,·)dΛ(ω)$$

where $c(ω,γ) = \exp(iω^\topγ) > 0$ and $ϕ(ω;θ) := E_X[ℳ(X;θ)\exp(iω^\topX)]$ is the Fourier transform (or characteristic function) of Borel measurable function $ℳ(x;θ)$.
relative to $P_X$. Hence, if supp$(\Lambda) = \mathbb{R}^d$, the uniqueness of $\mu_\theta$ follows from the uniqueness of $\phi(x; \theta)$. Bierens (1982) was the first to observe the characterization of the CMR in terms of the integral transform and used it to construct the consistent CM tests of functional form (cf. Section 5).

By Theorem 3.2, $\mu_\theta$ captures all information about $E[\psi(Z; \theta)|x]$ for every $x \in \mathcal{X}$ for which $P_X(x) > 0$. Consequently, estimation and inference on CMR can be performed by means of $\mu_\theta$ using the kernel arsenal. As mentioned earlier, for each $f \in \mathcal{F}$ and $\theta \in \Theta$, the inner product $\langle f, \mu_\theta \rangle_{\mathcal{F}} = (f, E[\xi \phi(X, Z)])_{\mathcal{F}}$ can be interpreted as a restriction of conditional moments with respect to $f$. Moreover, the investigator can inspect $\mu_\theta(x, z)$, which measures the extent to which the moment conditions are violated at $(x, z)$, i.e., structural instability, in order to understand the nature of misspecification.

### 3.2 Kernel Maximum Moment Restriction

Based on the CMME $\mu_\theta$, we can now define the MMR as

$$M(\theta) := \sup_{\|f\|_{\mathcal{F}} \leq 1} M_\theta f = \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_\theta \rangle_{\mathcal{F}} = \|\mu_\theta\|_{\mathcal{F}}.$$  \hspace{1cm} (8)

By Theorem 3.2, $M(\theta) \geq 0$ and $M(\theta) = 0$ if and only if $\theta = \theta_0$. Put differently, $M_\theta(\theta)$ measures how much the models associated with $\theta$ violate the original CMR in (1).

To obtain an expression for $M_\theta(\theta)$, we define a positive definite kernel $h_\theta : (\mathcal{X} \times \mathcal{Z}) \times (\mathcal{X} \times \mathcal{Z}) \rightarrow \mathbb{R}$ based on the feature map $\xi \phi : \mathcal{X} \times \mathcal{Z} \rightarrow \mathcal{F}^q$ as follows:

$$h_\theta((x, z), (x', z')) := \langle \xi \phi(x, z), \xi \phi(x', z') \rangle_{\mathcal{F}} = \psi(z; \theta) \psi(z'; \theta) h(x, x').$$  \hspace{1cm} (9)

Then, a closed-form expression for $M(\theta)$ in terms of the kernel $h_\theta$ follows straightforwardly.

**Theorem 3.3.** Assume that $E[h_\theta((X, Z), (X, Z))] < \infty$. Then,

$$M^2(\theta) = E[h_\theta((X, Z), (X', Z'))]$$

where $(X', Z')$ is independent copy of $(X, Z)$ with the same distribution.

Finally, the Mercer’s representation (3) of $k$ allows us to interpret $h_\theta$ and $M(\theta)$ in terms of a continuum of unconditional moment restrictions.

**Theorem 3.4.** Let $\{(\lambda_j, e_j)\}$ be eigenvalue/eigenfunction pairs associated with the kernel $k$ and $\xi \phi_\theta(x, z) := (\psi_1(z; \theta)e_j(x), \ldots, \psi_q(z; \theta)e_j(x))$. Then, for each $\theta \in \Theta$, $h_\theta((x, z), (x', z')) = \sum_j \lambda_j \xi \phi_\theta(x, z)^\top \xi \phi_\theta(x', z')$ and $M^2(\theta) = \sum_j \lambda_j \|E[\xi \phi_\theta(X, Z)]\|_2^2$.

That is, we can interpret $E[\xi \phi_\theta(X, Z)]$ as the UMR with $e_j$ acting as an instrument. Moreover, $M^2(\theta)$ can be viewed as a weighted sum of moment restrictions based on the sequence of weights and instruments $(\lambda_j, e_j)$. As a result, the CM test based on $M^2(\theta)$ as a test statistic examines an infinite number of moment restrictions. Note that $(\lambda_j, e_j)$ are implicitly defined by the choice of $k$. 

8
4 Kernel Conditional Moment Test

By virtue of Theorem 3.2, we can reformulate the CM testing problem (2) in terms of the test statistic $M^2(\theta)$ as

$$H_0 : M^2(\theta) = 0, \quad H_1 : M^2(\theta) \neq 0.$$  

Given an i.i.d. sample $\{(x_i, z_i)\}_{i=1}^n$ from the distribution $P_{XZ}$ and $h_\theta$ as defined in (9), we can estimate $M^2(\theta)$ by

$$\hat{M}^2_n(\theta) = \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h_\theta((x_i, z_i), (x_j, z_j)), \quad (10)$$

which is in the form of $U$-statistics (Serfling 1980; Section 5). Although there exist several potential estimators for $M^2(\theta)$, we focus on (10) as it is a minimum-variance unbiased estimator with appealing asymptotic properties (cf. Appendix B). Moreover, (10) also provides a basis for estimation of $\theta_0$ simply by minimizing $\hat{M}^2_n(\theta)$ with respect to $\theta \in \Theta$. Preliminary results on estimation problem are given in Appendix B.

Next, we characterize the asymptotic distributions of $\hat{M}^2_n(\theta)$ under the null and alternative hypotheses.

**Theorem 4.1.** Assume that $\mathbb{E}[h_\theta^2((X, Z), (X', Z'))] < \infty$ for all $\theta \in \Theta$. Let $U := (X, Z)$ and $U' := (X', Z')$. Then, the following statements hold:

1. If $\theta \neq \theta_0$, $\hat{M}^2_n(\theta)$ is asymptotically normal with

   $$\sqrt{n}(\hat{M}^2_n(\theta) - M^2(\theta)) \overset{d}{\to} \mathcal{N}(0, 4\sigma_n^2),$$

   where $\sigma_n^2 = \text{Var}_U[\mathbb{E}_{U'}[h_\theta(U, U')]]$.

2. If $\theta = \theta_0$, then $\sigma_n^2 = 0$ and

   $$n\hat{M}^2_n(\theta) \overset{d}{\to} \sum_{j=1}^\infty \lambda_j (W_j^2 - 1), \quad (11)$$

   where $W_j \sim \mathcal{N}(0, 1)$ and $\lambda_j$ is the solution of $\lambda_j \phi_j(u) = \int h(u, u')\phi_j(u') dP(u')$ for non-zero $\phi_j$.

As we can see, $n\hat{M}^2_n(\theta) < \infty$ with probability one under the null $\theta = \theta_0$ and diverts to infinity at a rate $\mathcal{O}(\sqrt{n})$ under any fixed alternative $\theta \neq \theta_0$. Hence, a consistent CM test can be constructed as follows: if $\gamma_{1-\alpha}$ is the $1 - \alpha$ quantile of the CDF of $n\hat{M}^2_n(\theta)$ under the null $\theta = \theta_0$, we reject the null with significance level $\alpha$ if $n\hat{M}^2_n(\theta) \geq \gamma_{1-\alpha}$.

**Proposition 4.1** (Arcones and Gine (1992); p. 671). Assume the conditions of Theorem 4.1. The test that rejects the null $\theta = \theta_0$ when $n\hat{M}^2_n(\theta) > \gamma_{1-\alpha}$ is consistent against any fixed alternative $\theta \neq \theta_0$, i.e., the limiting power of the test is one.

Unfortunately, the limiting distribution in (11) and its $1 - \alpha$ quantile do not have an analytic form. Following recent works on kernel-based tests (Liu et al. 2016, Chwialkowski et al. 2016, Gretton et al. 2012), we propose to approximate the
Algorithm 1 KCM Test with bootstrapping

Require: Bootstrap sample size $B$, significance level $\alpha$

for $t \in \{1, \ldots, B\}$ do
  Draw $(w_1, \ldots, w_n) \sim \text{Mult}(n; \frac{1}{n}, \ldots, \frac{1}{n})$
  $\hat{M}_n^* (\theta) = \sum_{i \neq j} (w_i/n - 1/n)(w_j/n - 1/n) h_\theta((x_i, z_i), (x_j, z_j))$
  $a_t \leftarrow n\hat{M}_n^* (\theta)$
end for

$\hat{\gamma}_{1-\alpha} := \text{empirical } (1-\alpha)-\text{quantile of } \{a_t\}_{t=1}^B$

Reject $H_0$ if $\hat{\gamma}_{1-\alpha} < n\hat{M}_n^2 (\theta)$ (see (10))

Critical values using the bootstrap method proposed by Arcones and Gine (1992), Huskova and Janssen (1993), which was also used in Liu et al. (2016). Specifically, we first draw multinomial random weights $(w_1, \ldots, w_n) \sim \text{Mult}(n; \frac{1}{n}, \ldots, \frac{1}{n})$ and calculate the bootstrap sample

$\hat{M}_n^* (\theta) = \sum_{1 \leq i \neq j \leq n} (w_i/n - 1/n)(w_j/n - 1/n) h_\theta((x_i, z_i), (x_j, z_j))$.

We then calculate the empirical quantile $\hat{\gamma}_{1-\alpha}$ of $n\hat{M}_n^2 (\theta)$. The consistency of $\hat{\gamma}_{1-\alpha}$ for degenerate $U$-statistics has been established (Arcones and Gine 1992, Huskova and Janssen 1993).

We summarize our bootstrap kernel conditional moment (KCM) test in Algorithm 1.

5 Related Work

Existing CM tests can generally be categorized into two classes. The former is based on a transformation of CMR into a continuum of unconditional counterparts, e.g., Bierens (1982; 1990), de Jong (1996), Bierens and Ploberger (1997), and Donald et al. (2003) to name a few. The latter employs nonparametric kernel estimation which includes Zheng (1996), Li and Wang (1998), Fan and Li (2000) among others. While both classes lead to consistent tests, they exhibit different asymptotic behaviors; see, e.g., Fan and Li (2000), Delgado et al. (2006) for detailed comparisons.

A continuum of unconditional moments. One of the classical approaches is to find a parametric weighting function $w(x, \eta)$ such that

$\mathbb{E}[\psi(Z; \theta)|X] = 0 \text{ a.s.} \iff \mathbb{E}[\psi(Z; \theta)w(X, \eta)] = 0$,

for almost all $\eta \in \Xi \subseteq \mathbb{R}^m$ where $\eta$ is a nuisance parameter. Newey (1985) and Tauchen (1985) proposed the so-called M-test using a finite number of weighting functions. Since it imposes only a finite number of moment conditions, the test cannot be consistent against all possible alternatives and power against specific alternatives depends on the choice of these weighting functions. de Jong (1996) and Donald et al. (2003) showed that this issue can be circumvented by allowing the number of moment conditions to grow with sample size. Although our KCM
test generally relies on an infinite moment conditions, one can impose finitely many conditions using the finite dimensional RKHS such as those endowed with linear and polynomial kernels or resorting to finite-dimensional kernel approximations.

Stinchcombe and White (1998) showed that there exists a wide range of \(w(x, \eta)\) that lead to consistent CM tests. They call these functions “totally revealing”. For instance, Bierens (1990) proposed the first consistent specification test for nonlinear regression models using \(w(x, \eta) = \exp(i\eta'^\top x)\) for \(\eta \in \mathbb{R}^d\). Similarly, Bierens (1990) used \(w(x, \eta) = \exp(\eta'^\top x)\) for \(\eta \in \mathbb{R}^d\). An indicator function \(w(x, \eta) = 1(\alpha^\top x \leq \beta)\) with \(\eta = (\alpha, \beta) \in \mathbb{S}^d \times (-\infty, \infty)\) where \(\mathbb{S}^d = \{\alpha \in \mathbb{R}^d : \|\alpha\| = 1\}\) was used in Escanciano (2006) and Delgado et al. (2006). Other popular weighting functions include power series, Fourier series, splines, and orthogonal polynomials, for example. In light of Theorem 3.4, the KCM test falls into this category where weighting functions are eigenfunctions associated with the kernel \(k\).

Since \(w(x, \eta)\) depends on the nuisance parameter \(\eta\), Bierens (1982) suggested to integrate \(\eta\) out, resulting in an integrated conditional moment (ICM) test statistic:

\[
\hat{T}_n(\theta) = \int_\Xi \|\hat{Z}_n(\eta)\|^2 d\nu(\eta),
\]

where \(\Xi\) is a compact subset of \(\mathbb{R}^d\), \(\nu(\eta)\) is a probability measure on \(\Xi\), and \(\hat{Z}_n(\eta) := (1/\sqrt{n}) \sum \psi(z; \theta) w(x, \eta)\). The limiting null distribution of the ICM test was proven to be a zero-mean Gaussian process (Bierens 1990). Bierens and Ploberger (1997) also characterizes the asymptotic null distribution of a general class of real-valued weighting functions.

The following theorem establishes the connection between the KCM and ICM test statistics.

**Theorem 5.1.** Let \(k(x, x') = \varphi(x - x')\) be a shift-invariant kernel on \(\mathbb{R}^d\). Then, we have

\[
M^2(\theta) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \|E[\psi(Z; \theta) \exp(i\omega^\top X)]\|^2_2 d\Lambda(\omega)
\]

where \(\Lambda\) is a Fourier transform of \(k\).

This theorem is quite insightful as it describes the KCM test statistic as the ICM test statistic of Bierens (1982) where the distribution on the nuisance parameter \(\omega\) is a Fourier transform of the kernel. For instance, the Gaussian kernel \(k(x, x') = \exp(-\|x - x'\|^2/2\sigma^2)\) corresponds to the Gaussian density \(\Lambda(\omega) = \exp(-\sigma^2\|\omega\|^2_2/2)\); see Muandet et al. (2017; Table 2.1) for more examples. Note that both weighting functions and integrating measures are determined implicitly by the kernel \(k\). Unlike ICM tests, KCM tests can be evaluated without solving the high-dimensional numerical integration (12) explicitly. Moreover, KCM tests can be easily generalized to \(\mathcal{X}\) that is not necessarily a subset of \(\mathbb{R}^d\).

Carrasco and Florens (2000) also considers a similar setting that involves a continuum of moment conditions in RKHS. Their approach, however, differs significantly from ours. First, they consider a specific case where the Hilbert space is a set of square integrable function of a scalar \(t \in [0, T]\) with the unconditional moment conditions \(E[\psi_t(X, \theta_0)] = 0\) for all \(t \in [0, T]\). Second, their key question is to identify the optimal choice of weighting matrix in GMM. Third, estimation is actually based on a truncation of infinite moment conditions. Lastly, they also proposed the CM test similar to the ICM tests, but it can handle only the case with \(Z \in \mathbb{R}\), while our test is applicable to any domain with a valid kernel.
Nonparametric kernel estimation. The second class of tests, known as smooth tests (Zheng 1996, Li and Wang 1998, Fan and Li 2000), adopts the statistic of the form

\[ T(\theta) = \mathbb{E}[\psi(Z; \theta)^\top \mathbb{E}[\psi(Z; \theta)|X]f(X)]. \]  

(13)

Based on the kernel estimator of \( \mathbb{E}[\psi(Z; \theta)|X]f(X) \), the empirical estimate of (13) can be expressed as

\[ \hat{T}_n(\theta) = \frac{1}{n(n-1)h^d} \sum_{1 \leq i \neq j \leq n} \psi(z_i; \theta)^\top \psi(z_j; \theta)K_{ij} \]  

(14)

where \( K_{ij} = K((x_i - x_j)/h), K(\cdot): \mathbb{R}^d \to \mathbb{R} \) is a normalized kernel function and \( h \) is a smoothing parameter. Here, we emphasize that existing smooth tests rely on the kernel density estimator (KDE) in which the kernel used is not necessarily a reproducing kernel; see, e.g., Scott (1992; Ch. 6) and Kim and Scott (2012). Nevertheless, if \( K(\cdot) \) is a reproducing kernel, the test statistic \( \hat{T}_n(\theta) \) with a fixed smoothing parameter \( h \) resembles the KCM test statistic (10). In fact, Fan and Li (2000) has shown that the ICM test is a special case of the kernel-based test with a fixed smoothing parameter. However, the critical drawback of the nonparametric kernel-based tests is that they have non-trivial power only against local alternatives that approach the null at a slower rate than \( 1/\sqrt{n} \), due to the slower rate of convergence of kernel density estimators, i.e., \( O((nh^{d/2})^{-1/2}) \) as \( h \to 0 \) (Fan and Li 2000). Moreover, these tests are susceptible to the curse of dimensionality.

Last but not least, the kernel estimator is also a key ingredient in empirical likelihood-based CM tests (Tripathi and Kitamura 2003, Kitamura et al. 2004, Dominguez and Lobato 2004).

Kernelized Stein discrepancy (KSD). Stein’s methods (Stein 1972) are among the most popular techniques in statistics and machine learning. One notable example is the Stein discrepancy which aims to characterize complex, high-dimensional distribution \( p(x) = \hat{p}(x)/N \) with intractable normalization constant \( N = \int \hat{p}(x)dx \) using a Stein operator \( A_p \) such that

\[ p = q \iff \mathbb{E}_{x \sim q}[A_p f(x)] = 0, \quad \forall f, \]  

(15)

where \( A_p f(x) := \nabla_x \log p(x)f(x)^\top + \nabla_x f(x) \). The Stein operator \( A_p \) depends on the density \( p \) through its score function \( s_p(x) := \nabla_x \log p(x) = \frac{\nabla \hat{p}(x)}{\hat{p}(x)} \), which is independent of \( N \). When \( p \neq q \), the expectation in (15) gives rise to a Stein discrepancy

\[ S(p, q) := \mathbb{E}_{x \sim q}[A_p f(x)] = \mathbb{E}_{x \sim q}[(s_p(x) - s_q(x))f(x)]. \]

See, also, Ley and Swan (2013) and Liu et al. (2016; Lemma 2.3). The Stein discrepancy has led to numerous applications such as variance reduction (Oates et al. 2017) and goodness-of-fit testing (Liu et al. 2016, Chwiałkowski et al. 2016), among others.

Like (4), we can observe that (15) is indeed a continuum of unconditional moment conditions. To make an explicit connection between Stein discrepancy and CMR, we need to assume access to the probability densities. Let \( \mathcal{P}_\Theta \) be a space of probability densities \( p(z; \theta) \) such that \( \theta \mapsto p(z; \theta) \) is injective. We choose
(d) REG-HOM (n = 100)  (e) REG-HET (n = 100)  (f) SIMEQ (n = 100)

Figure 2: The test powers of KCM, ICM, and smooth tests averaged over 300 trials as we vary the values of $n$ (top) and $\delta$ (bottom). Type-I errors of these tests are shown in Figure 3 in Appendix D. See main text for the interpretation.

$$\psi(z; \theta) = \nabla_z \log p(z; \theta) =: s_\theta(z)$$ as the associated score function.\(^2\) This yields the following CMR:

$$E[\nabla_z \log p(Z; \theta_0) \mid X] = 0, \quad P_X\text{-a.s.} \quad (16)$$

Then, for any $\theta \in \Theta$, it follows that $E[\psi(Z; \theta) f(X)] = E[s_\theta(Z)f(X) - s_{\theta_0}(Z)f(X)] = E[(s_\theta(Z) - s_{\theta_0}(Z))f(X)] =: \Delta(\theta, \theta_0)$. While $\Delta(\theta, \theta_0)$ resembles the Stein discrepancy, we highlight the key differences. First, this characterization requires that the model is correctly specified, i.e., $p(z; \theta)$ is observationally indistinguishable from the underlying data distribution. Second, like the Stein discrepancy, it can be interpreted as the $f(x)$-weighted expectation of the score difference $s_\theta - s_{\theta_0}$. In contrast, the weighting function $f(x)$ in our setting depends only on $X$, which is a subvector of $Z$. We provide further discussion about this discrepancy measure in Appendix A.

This theorem follows directly from the above observation.

**Theorem 5.2.** Let $\mathcal{P}_\Theta$ be a space of probability densities $p(z; \theta)$. Assume that $\theta \mapsto p(z; \theta)$ is injective and $\theta_0 \in \Theta$. If $\psi(z; \theta) = \nabla_z \log p(z; \theta)$ and $X = Z$, we have $S(p(z; \theta), p(z; \theta_0)) = \Delta(\theta, \theta_0)$.

\(^2\)This differs from the standard definition of score function as $\nabla_\theta \log p(z|\theta)$ in the interpretation of maximum likelihood as generalized method of moments (Hall 2005).
Mostly related to our work are the RKHS-based Stein’s methods \cite{liu2016kernel,chwialkowski2016approximate}. Specifically, if we assume the conditions of Theorem 5.2 and that \( f \) belongs to the RKHS, it follows that \( \Delta(\theta, \theta_0) \) coincides with the kernelized Stein discrepancy (KSD) proposed in Liu et al. \cite{liu2016kernel} and Chwialkowski et al. \cite{chwialkowski2016approximate}. We will elaborate this connection in further details in future work.

6 Experiments

We report the finite-sample performance of the KCM test against two well-known consistent CM tests, namely ICM test and smooth test, as discussed in Section 5. We evaluate all tests with a bootstrap size \( B = 1000 \) and a significance level \( \alpha = 0.05 \).

(1) **KCM**: The bootstrap KCM test using U-statistic in Algorithm 1. We use the RBF kernel with bandwidth chosen by the median heuristic.

(2) **ICM**: The test based on an integration over weighting functions. Following Stute \cite{stute1997test} and Delgado et al. \cite{delgado2006adaptive}, we use \( \psi(z_i; \theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(z_i; \theta) \mathbb{1}(x_i \leq x) \) where \( \mathbb{1}(\cdot) \) is an indicator function. The density \( \nu \) is chosen to be the empirical distribution of \( X \). This leads to a simple test statistic \( t_n = \sum_{i=1}^{n} r_n(x_i) \mathbb{1}(x_i \leq x) \) where \( r_n(x) := \frac{1}{n} \sum_{i=1}^{n} \psi(z_i; \theta) \mathbb{1}(x_i \leq x) \). We follow the bootstrap procedure in Delgado et al. \cite{delgado2006adaptive}; Sec. 4.3) to compute the critical values.

(3) **Smooth**: The test based on nonparametric kernel estimation. We use \( \psi(z_i; \theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(z_i; \theta) \mathbb{1}(x_i \leq x) \) with the kernel function chosen to be the standard Gaussian whose bandwidth is chosen by the rule-of-thumb \( h = \frac{n^{-1/5}}{5} \). The critical values are obtained using the same bootstrap procedure as in Delgado et al. \cite{delgado2006adaptive}; Sec. 4.2).

**Testing a regression function (REG).** We follow a similar simulation of regression model used in Lavergne and Nguimkeu \cite{lavergne2016testing}. In this setting, for a given estimate \( \tilde{\beta} \) of the regression parameters, the null hypothesis is

\[
H_0 : \mathbb{E}[Y - \tilde{\beta}^\top X | X] = 0 \quad \text{a.s.}
\]

where \( X \in \mathbb{R}^d \) and \( Y \) is a univariate random variable, i.e., \( Z = (Y, X) \). The data are generated from the data generating process (DGP):

\[
Y = \beta_0^\top X + e.
\]

We set \( \beta_0 = 1 \), and \( X \sim \mathcal{N}(0, I_d) \). For the error term \( e \), we consider two scenarios: (i) **Homoskedastic (HOM)**: \( e = e, e \sim \mathcal{N}(0, 1) \) and (ii) **Heteroskedastic (HET)**: \( e = \gamma \sqrt{0.1 + 0.1 ||X||^2} \). In each trial, we obtain an estimate of \( \beta_0 \) by \( \tilde{\beta} = \beta_0 + \gamma \) where \( \gamma \sim \mathcal{N}(0, \delta^2 I_d) \). In this experiment, we set \( d = 5 \). When \( \delta = 0 \), the model is correctly specified, whereas the model is misspecified, i.e., \( H_0 \) is false, if \( \delta \neq 0 \). Different values of \( \delta \) correspond to different degrees of deviation from the null.
Testing the simultaneous equation model (SIMEQ). Following Newey (1990) and Delgado et al. (2006), we consider the equilibrium model

\[ Q = \alpha_d P + \beta_d R + U, \quad \alpha_d < 0, \quad \text{(Demand)} \]
\[ Q = \alpha_s P + \beta_s W + V, \quad \alpha_s > 0, \quad \text{(Supply)} \]

where \( Q \) and \( P \) denote quantity and price, respectively, \( R \) and \( W \) are exogeneous variables, and \( U \) and \( V \) are the error terms. In this setting, \( Z = (Q, P, R, W) \) and \( X = (R, W) \). The null hypothesis can be expressed as

\[ H_0 : \mathbb{E} \left[ \begin{bmatrix} Q - \alpha_d P - \beta_d R \\ Q - \alpha_s P - \beta_s W \end{bmatrix} | X \right] = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \]

a.s. for some \( \theta_0 = (\alpha_d, \beta_d, \alpha_s, \beta_s) \). We generate data according to \( Q = \lambda_{11} R + \lambda_{12} W + V_1 \) and \( P = \lambda_{21} R + \lambda_{22} W + V_2 \) where \( R \) and \( W \) are independent standard Gaussian random variables while \( V_1 \) and \( V_2 \) are correlated standard Gaussian random variables with \( 1/\sqrt{2} \) covariance and independent of \( (R, W) \). We set \((\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}) = (-1, 1, 1, 1)\). The parameters \( \theta_0 \) are estimated using a two-stage least square (2SLS) procedure (Angrist and Pischke 2008; Ch. 4). The estimate \( \hat{\theta} \) is obtained as in the previous experiment. The null hypothesis corresponds to \( \delta = 0 \) and different values of \( \delta \) corresponds to alternative hypotheses. Rejecting \( H_0 \) means that the functional form of the supply and demand curves are misspecified.

Figure 2 depicts the empirical results for \( n \in \{20, 50, 100, 200, 500, 1000\} \) and \( \delta \in \{0.001, 0.01, 0.05, 0.1\} \). First, it can be observed that KCM, ICM, and smooth tests are all capable of detecting the misspecification as the sample size and \( \delta \) are sufficiently large. Second, the KCM test tends to outperform both ICM and smooth tests in terms of the test power, especially in a low sample regime (see Figure 2a–2c) and a small deviation regime (see Figure 2d–2f). In addition, the smooth test tends to also outperform the ICM test. We believe that this may be because of the choice of weighting function and the integrating measure, which give us a simple ICM test statistic. With appropriate choice of these parameters, we expect the ICM test to perform better (see Theorem 5.1). The ICM test statistic also appears to be more conservative than the KCM and smooth tests as is evident from the Type-I error in Figure 3.

7 Conclusion

To conclude, we propose a new conditional moment test called the KCM test whose statistic is based on a novel representation of the conditional moment restrictions in a reproducing kernel Hilbert space. This representation captures all necessary information about the original conditional moment restrictions. Hence, the resulting test is consistent against all fixed alternatives, is easy to use in practice, and also has connections to existing tests in the literature. It also has an encouraging finite-sample performance compared to those tests. While the conditional moment restrictions have a long history in econometrics and so does the concept of reproducing kernel Hilbert spaces in machine learning, the intersection of these concepts remains unexplored. We believe that this work gives rise to a new and promising framework for conditional moment restrictions which constitute numerous applications in econometrics, causal inference, and machine learning.
Despite our promising results, there remain several open questions still to be answered and limitations to be overcome. First, it is crucial to consider the parameter estimation based on the CMR and understand how it affects the performance of the subsequent CM test. Second, it is natural to extend our framework via a general vector-valued RKHS which will allow for more flexibility in modelling the CMR. Third, an extension of our framework to semi-parametric and nonparametric settings will also make it more applicable to real-world econometric problems. Last but not least, we also plan to evaluate our framework on other realistic scenarios.

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A  Conditional Moment Discrepancy (CMMD)

The kernel MMR can also be used to define a discrepancy measure between different models based on the CMR. Let $\mathcal{M}_{\theta_1}$ and $\mathcal{M}_{\theta_2}$ be two models parameterized by $\theta_1, \theta_2 \in \Theta$, respectively. Then, we can define a CMR-based discrepancy measure between these two models as follows.

**Definition A.1.** For $\theta_1, \theta_2 \in \Theta$, we define a conditional moment discrepancy as $\Delta(\theta_1, \theta_2) := \|\mu_{\theta_1} - \mu_{\theta_2}\|_{F_r}$.

By Theorem 3.2, $\Delta(\theta_1, \theta_2) \geq 0$ and $\Delta(\theta_1, \theta_2) = 0$ if and only if the two models $\mathcal{M}_{\theta_1}$ and $\mathcal{M}_{\theta_2}$ are indistinguishable in terms of the CMR alone. Moreover, if the global identifiability (A3) holds, $\Delta(\theta_0, \theta) = M(\theta)$ for all $\theta \in \Theta$ by the definition of $\theta_0$. Since $\Delta(\theta_1, \theta_2) = \|E[\xi_{\theta_1}(X, Z) - \xi_{\theta_2}(X, Z)]\|_{F_r}^2 = \|E[\xi(X, Z)]\|_{F_r}^2$

where $\bar{\xi}(x, z) := \xi_{\theta_1}(x, z) - \xi_{\theta_2}(x, z) = (\psi(z; \theta_1) - \psi(z; \theta_2))k(x, \cdot)$, the CMMD is the CMME defined on the function $\psi(z; \theta_1) - \psi(z; \theta_2)$, which we call a differential residual function. As a result, $\Delta(\theta_1, \theta_2)$ also has a close-form expression similar to that in Theorem 3.3.

**Corollary A.1.** Let

$h((x, z), (x', z')) := (\psi(z; \theta_1) - \psi(z; \theta_2))^\top (\psi(z'; \theta_1) - \psi(z'; \theta_2))k(x, x')$

and assume that $E[h((X, Z), (X, Z))] < \infty$. Then, we have

$\Delta^2(\theta_1, \theta_2) = E[h((X, Z), (X', Z'))]$ where $(X', Z')$ is an independent copy of $(X, Z)$ with an identical distribution.

**Proof.** The result follows by applying the proof of Theorem 3.3 to the feature map $\bar{\xi}(x, z) := \xi_{\theta_1}(x, z) - \xi_{\theta_2}(x, z) = (\psi(z; \theta_1) - \psi(z; \theta_2))k(x, \cdot)$.

Furthermore, we can express the empirical CMMD as

$\Delta_n^2(\theta_1, \theta_2) := \frac{1}{n(n - 1)} \sum_{1 \leq i \neq j \leq n} h((x_i, z_i), (x_j, z_j))$

where $h((x, z), (x', z')) := (\psi(z; \theta_1) - \psi(z; \theta_2))^\top (\psi(z'; \theta_1) - \psi(z'; \theta_2))k(x, x')$.

As we can see, the RKHS norm, inner product, and function evaluation computed with respect to $\mu_{\theta}$ all have a meaningful economic interpretations which we summarize in Table 1.

B  Parameter Estimation

Besides hypothesis testing, another important application of the CMR is parameter estimation. That is, given the CMR as in (1), we aim to find a good estimate of $\theta_0$ that satisfies (1) from the observed data $\{(x_i, z_i)\}_{i=1}^n$. Based on the MMR, we define the estimator of $\theta_0$ as the parameter that minimizes (10), i.e.,

$\hat{\theta}_n := \arg \min_{\theta \in \Theta} \hat{M}^2_n(\theta) = \arg \min_{\theta \in \Theta} \frac{1}{n(n - 1)} \sum_{1 \leq i \neq j \leq n} h_\theta((x_i, z_i), (x_j, z_j))$.  

(17)
Table 1: An interpretation of different operations on $\mu_\theta$ in $F_q$.

| Operation | Interpretation |
|-----------|----------------|
| $\|\mu_\theta\|_{F_q}$ | conditional moment violation |
| $\langle f, \mu_\theta \rangle_{F_q}$ | violation w.r.t. the instrument $f$ |
| $\mu_\theta(x, z)$ | structural instability at $(x, z)$ |
| $\|\mu_{\theta_1} - \mu_{\theta_2}\|_{F_q}$ | discrepancy between $M_{\theta_1}$ and $M_{\theta_2}$ |

We call $\hat{\theta}_n$ a minimum maximum moment restriction (MMMR) estimate of $\theta_0$. Previously, Lewis and Syrgkanis (2018) and Bennett et al. (2019) proposed to estimate $\theta_0$ based on (5) and $F_q$ that is parameterized by deep neural networks. However, their algorithms require solving a minimax game, whereas our approach for estimation is merely a minimization problem.

The following theorem shows that $\hat{\theta}_n$ is a consistent estimate of $\theta_0$. The proof can be found in Appendix C.6.

**Theorem B.1** (Consistency of $\hat{\theta}_n$). Assume that the parameter space $\Theta$ is compact. Then, we have $\hat{\theta}_n \overset{p}{\to} \theta_0$.

Despite the consistency, we suspect that $\hat{\theta}_n$ may not be asymptotically efficient and there exist better estimators. Theorem 3.4 shows that $M(\theta)$ depends on a continuum of moment conditions reweighted by the non-uniform eigenvalues $(\lambda_j)$, which suggests that a reweighting matrix must also be incorporated in order to achieve the optimality (Hall 2005). Constructing an optimal choice of reweighting matrix in an infinite dimensional RKHS is an interesting topic (Carrasco and Florens 2000), and we leave it to future work.

C Proofs

This section collects all the proofs of the results presented in the main paper.

C.1 Proof of Lemma 3.1

**Proof.** We have $M_{\theta_0}f = \sum_{i=1}^q \mathbb{E}[\psi_i(Z; \theta_0)f_i(X)]$ and, for all $i = 1, \ldots, q$,

$$
\mathbb{E}_{XZ}[\psi_i(Z; \theta_0)f_i(X)] = \mathbb{E}_X[\mathbb{E}_Z[\psi_i(Z; \theta_0)f_i(X)|X]] = \mathbb{E}_X[\mathbb{E}_Z[\psi_i(Z; \theta_0)|X]f_i(X)] = 0
$$

by the law of iterated expectation. The last equality follows from the definition of $\theta_0$ and the continuity of $f_i$, i.e., by Assumption (A4).

C.2 Proof of Theorem 3.1

**Proof.** Treating $\hat{\mu}_\theta$ as a sum of random variables $\xi_\theta(X_1, Z_1), \ldots, \xi_\theta(X_n, Z_n)$ in Banach space, the result follows directly from Pinelis (1994). It remains to show that, for each $\theta \in \Theta$, there exists a constant $C_\theta < \infty$ such that $||\xi_\theta(X, Z)||_{F_q} < C_\theta$ almost surely. Note that for any $(x, z) \in X \times Z$ for which $P_{XZ}(x, z) > 0$,

$$
||\xi_\theta(x, z)||_{F_q} = \sqrt{||\xi_\theta(x, z)||_{F_q}^2}
$$
3.3 Theorem 4.49, we have

\[ \sup_{x,z} \sqrt{\psi(z;\theta)^T \psi(z;\theta) k(x, x)} < \infty, \]

where the last inequality follows from Assumptions (A2) and (A4). Setting \( C_\theta = \sup_{x,z} \sqrt{\psi(z;\theta)^T \psi(z;\theta) k(x, x)} \) yields the result. \( \square \)

### C.3 Proof of Theorem 3.2

**Proof.** If \( \mathcal{M}(x; \theta_1) = \mathcal{M}(x; \theta_2) \) for \( P_X \)-almost all \( x \), then the equality \( \mu_{\theta_1} = \mu_{\theta_2} \) follows straightforwardly. Suppose that \( \mu_{\theta_1} = \mu_{\theta_2} \) and let \( \delta(x) := \mathcal{M}(x; \theta_1) - \mathcal{M}(x; \theta_2) \). Then, we have

\[
\| \mu_{\theta_1} - \mu_{\theta_2} \|^2_{\mathcal{F}_X} = \left\| \int \xi_{\theta_1}(x, z) dP_{XZ}(x, z) - \int \xi_{\theta_2}(x, z) dP_{XZ}(x, z) \right\|^2_{\mathcal{F}_X} \\
= \left\| \int \mathcal{M}(x; \theta_1) k(x, \cdot) dP_X(x) - \int \mathcal{M}(x; \theta_2) k(x, \cdot) dP_X(x) \right\|^2_{\mathcal{F}_X} \]

\[
= \left\| \int (\mathcal{M}(x; \theta_1) - \mathcal{M}(x; \theta_2)) k(x, \cdot) dP_X(x) \right\|^2_{\mathcal{F}_X} \]

\[
= \iint \delta(x)^T k(x, x') \delta(x') dP_X(x) dP_X(x') = 0, \tag{18}
\]

where \( X' \) is an independent copy of \( X \). It follows from (18) and Assumption (A2) that the function \( g(x) := \delta(x) p_X(x) \) has a zero L2-norm, i.e., \( \|g\|_2^2 = 0 \) where \( p_X \) denotes the density of \( P_X \). As a result, \( \delta(x) = 0 \) a.e. \( P_X \) implying that \( P_X(B_0) = 1 \) where \( B_0 := \{ x \in \mathcal{X} : \mathcal{M}(x; \theta_1) = \mathcal{M}(x; \theta_2) = 0 \} \). Therefore, \( \mathcal{M}(x; \theta_1) = \mathcal{M}(x; \theta_2) \) for \( P_X \)-almost all \( x \), as required. \( \square \)

### C.4 Proof of Theorem 3.3

**Proof.** By the definition of \( \mathbb{M}(\theta) \) and the Bochner integrability of \( \xi_{\theta} \),

\[
\mathbb{M}^2(\theta) = \| \mu_{\theta} \|^2_{\mathcal{F}_X} \\
= \langle \mu_{\theta}, \mu_{\theta} \rangle_{\mathcal{F}_X} \\
= \langle \mathbb{E}[\xi_{\theta}(X, Z)], \mathbb{E}[\xi_{\theta}(X, Z)] \rangle_{\mathcal{F}_X} \\
= \mathbb{E}[\langle \xi_{\theta}(X, Z), \xi_{\theta}(X, Z) \rangle_{\mathcal{F}_X}] \\
= \mathbb{E}[\langle \xi_{\theta}(X, Z), \xi_{\theta}(X', Z') \rangle_{\mathcal{F}_X}] \\
= \mathbb{E}[h_{\theta}(X, Z), (X', Z')],
\]

where \( (X', Z') \) is an independent copy of \( (X, Z) \) with an identical distribution. \( \square \)

### C.5 Proof of Theorem 3.4

**Proof.** By Mercer’s theorem (Steinwart and Christmann 2008; Theorem 4.49), we have

\[ k(x, x') = \sum_j \lambda_j e_j(x) e_j(x') \]

where the convergence is absolute and uniform. Recall that \( \xi_{\theta}^q(x, z) := (\psi_1(z; \theta), \ldots, \psi_q(z; \theta)) \). Hence, we can express the kernel \( h_{\theta} \) as

\[
h_{\theta}(x, z, (x', z')) = \psi(z; \theta)^T \psi(z'; \theta) k(x, x')
\]

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\[
\psi(z; \theta) = \psi(z'; \theta) \left( \sum_j \lambda_j e_j(x) e_j(x') \right)
\]
\[
= \sum_j \lambda_j \psi(z; \theta)^T \psi(z'; \theta) e_j(x) e_j(x')
\]
\[
= \sum_j \lambda_j [\psi(z; \theta) e_j(x)]^T [\psi(z'; \theta) e_j(x')]
\]
\[
= \sum_j \lambda_j \zeta_j(x, z)^T \zeta_j(x', z').
\]

Since \( \lambda_j > 0 \), the function \( h_\theta \) is positive definite. Then, we can express \( M^2(\theta) \) as follows:
\[
M^2(\theta) = \mathbb{E} [h_\theta((X, Z), (X', Z'))]
\]
\[
= \mathbb{E} \left[ \sum_j \lambda_j \zeta_j(X, Z)^T \zeta_j(X', Z') \right]
\]
\[
= \sum_j \lambda_j \mathbb{E}_{XZ} \left[ \zeta_j(X, Z)^T \mathbb{E}_{XZ} \left[ \zeta_j(X', Z') \right] \right]
\]
\[
= \sum_j \lambda_j \left\| \mathbb{E}_{XZ} \left[ \zeta_j(X, Z) \right] \right\|_2^2.
\]

This completes the proof. \( \square \)

### C.6 Proof of Theorem B.1

In order to show the consistency of \( \hat{\theta}_n := \text{arg min}_{\theta \in \Theta} \hat{M}^2_n(\theta) \), we need the uniform consistency of \( \hat{M}^2_n(\theta) \) and the continuity of \( \theta \mapsto M^2(\theta) \). The following lemma gives these two results.

**Lemma C.1.** Assume that there exists an integrable and symmetric function \( F_\psi \) such that \( \| \psi(z, \theta) \|_2 \leq F_\psi(z) \) for any \( \theta \in \Theta \) and \( z \in \mathcal{Z} \). If Assumptions (A4) holds, \( \sup_{\theta \in \Theta} |M^2_n(\theta) - M^2(\theta)| = 0 \) and \( \theta \mapsto M^2(\theta) \) are continuous.

**Proof.** Recall that
\[
M^2(\theta) = \mathbb{E} [h_\theta((X, Z), (X', Z'))]
\]
\[
\hat{M}^2_n(\theta) = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} h_\theta((x_i, z_i), (x_j, z_j)),
\]

where \( h_\theta((x, z), (x', z')) = \langle \xi_\theta(x, z), \xi_\theta(x', z') \rangle_{\mathcal{F}_\psi} = \psi(z; \theta)^T \psi(z'; \theta) k(x, x') \). Then, it follows that
\[
|h_\theta((x, z), (x', z'))| = |\langle \xi_\theta(x, z), \xi_\theta(x', z') \rangle_{\mathcal{F}_\psi}|
\]
\[
\leq \| \xi_\theta(x, z) \|_{\mathcal{F}_\psi} \cdot \| \xi_\theta(x', z') \|_{\mathcal{F}_\psi}
\]
\[
= \sqrt{\psi(z; \theta)^T \psi(z; \theta) k(x, x)} \sqrt{\psi(z'; \theta)^T \psi(z'; \theta) k(x', x')}
\]

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\[ = \|\psi(z; \theta)\|_2 \|\psi(z'; \theta)\|_2 \sqrt{k(x, x)k(x', x')} \]
\[ \leq F_\psi(z)F_\psi(z') \sqrt{k(x, x)k(x', x')} , \]
where \( F_\psi \) is an integrable and symmetric function. By Assumption (A4), \((x, x') \mapsto \sqrt{k(x, x)k(x', x')}\) is also an integrable function. Hence, \( \frac{\Delta}{\theta} \) is integrable. Since \( \Theta \) is compact, it then follows from Newey and McFadden (1994; Lemma 2.4) that \( \sup_{\theta \in \Theta} |\tilde{M}_n^2(\theta) - M^2(\theta)| \overset{\mathcal{D}}{\rightarrow} 0 \) and \( \theta \mapsto M^2(\theta) \) is continuous.

Now, we are in the position to present the proof of Theorem B.1.

**Proof of Theorem B.1.** By Assumption (A3) and Theorem 3.2, \( M^2(\theta) = 0 \) if and only if \( \theta = \theta_0 \). Thus \( M^2(\theta) \) is uniquely minimized at \( \theta_0 \). Since \( \Theta \) is compact, \( M^2(\theta) \) is continuous and \( \tilde{M}_n^2(\theta) \) converges uniformly in probability to \( M^2(\theta) \) by Lemma C.1. Then, \( \tilde{\theta}_n \overset{\mathcal{D}}{\rightarrow} \theta_0 \) by Newey and McFadden (1994; Theorem 2.1).

C.7 Proof of Theorem 4.1

**Proof.** First, we need to check that \( \sigma_n^2 \neq 0 \) when \( \theta \neq \theta_0 \) and \( \sigma_0^2 = 0 \) when \( \theta = \theta_0 \). Then, the results follow directly from Serfling (1980; Sec. 5.5.1 and Sec. 5.5.2).

Note that \( E_u[h_\theta(u, u')] = E_u[|\xi_\theta(u), \xi_\theta(u')|] = \langle \xi_\theta(u), E_u[\xi_\theta(u')] \rangle = \langle \xi_\theta(u), \mu_\theta \rangle = M_\theta \xi_\theta(u) \). When \( \theta = \theta_0 \), it follows that \( E_u[h_\theta(u, u')] = 0 \) by Lemma 3.1, and hence \( \sigma_n^2 = 0 \).

Next, suppose that \( \theta \neq \theta_0 \). Then, \( E_u[h_\theta(u, u')] = M_\theta \xi_\theta(u) = c(u) \). Since \( \sigma_n^2 = \text{Var}_u[c(u)] = E_u[(c(u) - E_u[c(u)])^2] \), \( \sigma_n^2 = 0 \) if and only if \( c(u) \) is a constant function. Note that we can write \( c(u) = c(x, z) = E_x Z_\theta [\psi(Z'; \theta)^\top \psi(z; \theta)k(x, X')] \). Therefore, by Assumptions (A3) and (A4), \( c(u) \) is not a constant function, implying that \( \sigma_n^2 > 0 \).

C.8 Proof of Theorem 5.1

**Proof.** Since the kernel \( k(x, x') = \varphi(x - x') \) is a shift-invariant kernel on \( \mathbb{R}^d \), it follows from Theorem 2.1 that
\[ \varphi(x - x') = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{-i(x - x')^\top \omega} \, d\Lambda(\omega). \]

Therefore, we can express \( M^2(\theta) \) as
\[
M^2(\theta) = E[\psi(Z; \theta)^\top \psi(Z'; \theta)k(X, X')] \\
= E[\psi(Z; \theta)^\top \psi(Z'; \theta)\varphi(X - X')] \\
= (2\pi)^{-d/2} E \left[ \psi(Z; \theta)^\top \psi(Z'; \theta) \left( \int_{\mathbb{R}^d} e^{-i(X - X')^\top \omega} \, d\Lambda(\omega) \right) \right] \\
= (2\pi)^{-d/2} E \left[ \psi(Z; \theta)^\top \psi(Z'; \theta) \left( \int_{\mathbb{R}^d} e^{-i\omega^\top X} e^{i\omega^\top X'} \, d\Lambda(\omega) \right) \right] \\
= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \psi(Z; \theta)^\top \psi(Z'; \theta) e^{-i\omega^\top X} e^{i\omega^\top X'} \, d\Lambda(\omega) \\
= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \left[ \psi(Z; \theta) e^{-i\omega^\top X} \right]^\top \left[ \psi(Z'; \theta) e^{i\omega^\top X'} \right] \, d\Lambda(\omega)
\]

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\[
= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \mathbb{E} \left[ \psi(Z; \theta) e^{-i\omega^T X} \right] \mathbb{E} \left[ \psi(Z'; \theta) e^{i\omega^T X'} \right] d\Lambda(\omega)
\]

\[
= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \left\| \mathbb{E} \left[ \psi(Z; \theta) \exp(i\omega^T X) \right] \right\|_2^2 d\Lambda(\omega).
\]

This completes the proof. \qed

\section{Type-I Error}

Our KCM test with bootstrapping is based on the asymptotic distribution of the test statistic under \( H_0 \) (cf. Theorem 4.1). Hence, the test reliably controls the Type-I error when the sample size is sufficiently large, i.e., we are in the asymptotic regime. For the considered examples, this is the case already for moderate sample sizes of \( n \approx 500 \). We report the Type-I error at a significant level \( \alpha = 0.05 \) for \( n \in \{20, 50, 100, 500, 1000\} \) in Figure 3 below.

![Figure 3: The Type-I errors averaged over 2000 trials of KCM, ICM, and smooth tests under the null hypothesis (\( \delta = 0 \)) as we vary the sample size \( n \).](image)