

Testing the Conditional Mean Independence for Functional Data

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SUMMARY

We propose a new nonparametric conditional mean independence test for a response variable Y and a predictor variable X where either or both can be function-valued. Our test is built on a new metric, the so-called functional martingale difference divergence (FMDD), which fully characterizes the conditional mean dependence of Y given X and extends the MDD proposed in Shao and Zhang (2014). We define an unbiased estimator of FMDD by using a \mathcal{U} -centering approach, and obtain its limiting null distribution under mild assumptions. Since the limiting null distribution is not pivotal, we adopt the wild bootstrap method to estimate the critical value and show the consistency of the bootstrap test. Our test can detect the local alternative which approaches the null at the rate of $n^{-1/2}$ with a nontrivial power, where n is the sample size. Unlike the recent three tests developed by Kokoszka et al (2008), Lei (2014), and Patilea et al. (2016), our test does not require a finite dimensional projection nor assume a linear model, and it does not involve any tuning parameters. Promising finite sample performance is demonstrated via simulations and a real data illustration in comparison with the existing tests.

Some key words: Functional Data; Nonlinear Dependence; U-statistic; Wild Bootstrap.

1. INTRODUCTION

Functional data analysis (FDA) has emerged as an important area of statistics which provides convenient and informative tools for the analysis of data objects of high or infinite dimension. It is generally applicable to problems which are difficult to cast into a framework of scalar or vector observations. In many situations, even if standard scalar or vector based approaches are applicable, functional data based approaches can often provide a more natural and parsimonious description of the data, and lead to more accurate inference and prediction. The area of FDA

has been growing rapidly in the recent decade since Ramsay and Silverman's (2005) excellent monograph, which provides a systematic account of the existing methodologies and tools to deal with data of functional nature; see Ferraty and Vieu (2006), Horváth and Kokoszka (2012), and Kokoszka and Reimherr (2017) for recent book-length treatments of FDA.

In the literature, functional linear models with a scalar or functional response Y and functional or vector covariates X have been extensively studied; see, e.g., Cuevas, Febrero, and Fraiman (2002), Cardot, Ferraty, Mas, and Sarda (2003), Chiou, Müller, and Wang (2004), Müller and Stadtmüller (2005), Yao, Müller, and Wang (2005a, 2005b), Cai and Hall (2006), Chiou and Müller (2007), among others. There have also been extensions of nonparametric regression models and inference to a functional data; see, e.g., Ferraty et al. (2011), Lian (2011), and Ferraty, Van Keilegom, and Vieu (2012). Most of the above-mentioned papers focus on modeling the conditional mean of the response variable Y given the covariates X using either linear models or nonparametric models. An important problem in conditional mean modeling is to assess whether X contributes to the conditional mean of Y , i.e., whether we have enough evidence to reject the following null hypothesis

$$H_0 : E(Y | X) = E(Y), \text{ almost surely}$$

based on a random sample $(X_i, Y_i)_{i=1}^n$. If H_0 is supported by the data, then there is no need to pursue a regression model for the mean of Y given X . In this paper, we shall address this testing problem when both Y and X can be either function-valued or vector-valued. It is worth noting that our test can be extended to do diagnostic checking for functional linear models; see Section 5 for more discussions.

To the best of our knowledge, the above testing problem has been first investigated by Kokoszka, Maslova, Sojka, and Zhu (2008) for a functional response and a functional covariate. Specifically, they assumed a functional linear model, i.e., $Y(t) = \int_0^1 \varphi(t, s)X(s)ds + \epsilon(t)$, $t \in [0, 1]$, where $\epsilon(\cdot)$ is an error process that is independent of the covariates and $\varphi(\cdot, \cdot)$ is a square integrable function on $[0, 1] \times [0, 1]$. They proposed a χ^2 -based test for the nullity of the φ , i.e., $H_0 : \varphi(s, t) = 0, \forall s, t$, which implies conditional mean independence of Y given X under the linear model assumption. Their procedure relies on the use of functional principal component analysis (FPCA) for both X and Y , and their test statistic measures the correlation of the finite-dimensional scores of X and Y . More recently, Patilea, Sánchez-Sellero, and Saumard (2016) introduced a nonparametric test for the predictor effect on a functional response allowing covariates to be either function-valued or vector-valued. Their test is nonparametric in the sense that no linear model assumption is imposed, but it requires the choice of 5 user-chosen quantities when X is function-valued and its implementation seems quite complex. Similar to Kokoszka et al. (2008), their test also projects the functional data to a finite dimensional space and constructs test statistics via the finite dimensional projections. Thus these two existing tests may have low power when the dependence of Y on X is along the directions that are orthogonal to the ones used. In the framework of a functional linear model with a scalar response and a functional covariate, Lei (2014) proposed the so-called exponential scan (ES) test to test a global linear effect by simultaneously testing the slope vectors in a sequence of functional principal components regression models and showed that their test is uniformly powerful over a certain class of smooth alternatives when the signal to noise ratio exceeds the detection boundary. Note that ES test also involves the use of FPCA and several user-chosen quantities and it requires strong Gaussian assumption on the error distribution. In the related diagnostic checking problem for functional linear models with a functional response and functional covariates, Chiou and Müller (2007) proposed a randomization test and recommended to use residual plots based on functional principal component scores of residual processes for diagnostic purposes; Gabrys, Horváth, and

Kokoszka (2010) proposed a goodness-of-fit test statistics that aim to detect a serial correlation in the error. Moreover, there are methods developed to do inference for the slope function for a scalar response and functional covariates; see Cardot et al. (2003), González-Manteiga and Martínez-Calvo (2011), among others.

In this article, we shall introduce a new nonparametric test to test H_0 versus

$$H_1 : \text{pr}\{E(Y | X) = E(Y)\} < 1,$$

where both the response Y and the covariate X can be either function-valued or vector-valued. The main contribution of our work lies in the following aspects: (1) we first generalize the martingale difference divergence (MDD) (Shao and Zhang, 2014; Park, Shao, and Yao, 2015), which characterizes the conditional mean independence of Y given X when both X and Y are vector-valued, to the functional setting. Note that MDD can be viewed as an analogue of distance covariance (Székely, Rizzo, and Bakirov, 2007), which measures the (in)dependence of two random vectors. The so-called functional martingale difference divergence (FMDD) is shown to fully characterize the conditional mean independence based on certain results developed by Lyons (2013), who extended the distance covariance from the Euclidean space to a metric space. (2) We then define the \mathcal{U} -centering (Székely and Rizzo, 2014) based sample estimate of FMDD, which is shown to be unbiased, and its limiting null distribution is shown to be nonpivotal; (3) We propose a wild bootstrap approach to approximate the limiting null distribution, and the asymptotic behavior of the bootstrap test statistic is carefully studied under both the null and alternatives. In particular, bootstrap consistency under the null and the limiting power under the local alternative that is in the n^{-a} , $a > 0$ neighborhood of the null hypothesis is derived. An appealing feature of our test is that there is no tuning parameter nor involves an user-chosen number, and the test does not impose any linear or parametric model assumptions so the new test is model-free. Through numerical simulations, we show that our test has an accurate size and a fairly high power relative to the tests developed by Kokoszka et al. (2008), Lei (2014), and Patilea et al. (2016).

We introduce some notation. Let $i = (-1)^{1/2}$ be the imaginary unit and $\mathcal{L}_2(\mathcal{I})$ be the separable Hilbert space consisting of all square integrable curves defined on $\mathcal{I} = [0, 1]$ with the inner product $\langle f, g \rangle = \int_{\mathcal{I}} f(u)g(u)du$ for $f, g \in \mathcal{L}_2(\mathcal{I})$. Also the vector product of vectors x and y is denoted by $\langle x, y \rangle = x^T y$. For a complex-valued function $f(\cdot)$, the complex conjugate of f is denoted by \bar{f} and $|f|^2 = \langle f, \bar{f} \rangle$. Denote the Euclidean norm (complex norm) of $x = (x_1, \dots, x_p) \in \mathbf{C}^p$ as $|x|$, where $|x|^2 = \langle x, \bar{x} \rangle = x_1 \bar{x}_1 + \dots + x_p \bar{x}_p$, and if $x \in \mathcal{L}_2(\mathcal{I})$, it is denoted as $|x|$, where $|x|^2 = \langle x, x \rangle$.

2. FUNCTIONAL MARTINGALE DIFFERENCE DIVERGENCE

To introduce the new metric FMDD for the functional data, we shall provide a brief review of the MDD. For $U \in \mathbb{R}^q$ and $V \in \mathbb{R}^p$, where q and p are fixed positive integers, Shao and Zhang (2014) proposed the so-called martingale difference divergence (MDD) to measure the conditional mean (in)dependence of V on U , i.e.,

$$E(V | U) = E(V), \text{ almost surely.} \quad (1)$$

Specifically $\text{MDD}(V | U)$ is defined as a nonnegative number that satisfies

$$\text{MDD}(V | U)^2 = \frac{1}{c_q} \int_{\mathbb{R}^q} \frac{|g_{V,U}(s) - g_V g_U(s)|^2}{|s|^{1+q}} ds, \quad (2)$$

where $g_{V,U}(s) = E(V e^{i\langle s, U \rangle})$, $g_V = E(V)$, $g_U(s) = E(e^{i\langle s, U \rangle})$, and $c_q = \pi^{(1+q)/2} / \Gamma\{(1+q)/2\}$. A key property is that $\text{MDD}(V | U)^2 = 0$ if and only if (1) holds, thus it completely

110 characterizes the conditional mean independence of V on U . Furthermore, if $E(|V| + |U|) < \infty$ and $E\{|U - E(U)||V - E(V)|\} < \infty$, then

$$\text{MDD}(V | U)^2 = -E\{[V - E(V)]^T [V' - E(V')] | U - U'\}, \quad (3)$$

where (V', U') is an independent copy of (V, U) .

115 Considering the definition of MDD in (3), we naturally define an analogue of MDD that is well defined for a functional response Y or a functional covariate X by replacing the vector product with the inner product associated with the separable Hilbert space, e.g., $\mathcal{L}_2(\mathcal{I})$. Note that Y and X are in metric spaces $(\mathcal{L}_y, |\cdot|_y)$ and $(\mathcal{L}_x, |\cdot|_x)$, respectively, i.e., $Y \in \mathcal{L}_y$, $X \in \mathcal{L}_x$. Throughout the paper, $(\mathcal{L}_y, \mathcal{L}_x)$ can be $(\mathcal{L}_2(\mathcal{I}), \mathcal{L}_2(\mathcal{I}))$ or $(\mathbb{R}^p, \mathbb{R}^q)$ or $(\mathcal{L}_2(\mathcal{I}), \mathbb{R}^q)$ or $(\mathbb{R}^p, \mathcal{L}_2(\mathcal{I}))$. Moreover, if either \mathcal{L}_y or \mathcal{L}_x is $\mathcal{L}_2(\mathcal{I})$, $|f|_x$ or $|f|_y$ is defined as $\{\int_{\mathcal{I}} f(u)^2 du\}^{1/2}$, otherwise it is the Euclidean norm. For the convenience of presentation, we do not distinguish between $|\cdot|_y$ and $|\cdot|_x$ but use $|\cdot|$ for both cases.

120 **DEFINITION 1 (FUNCTIONAL MARTINGALE DIFFERENCE DIVERGENCE).** For $Y \in \mathcal{L}_y$ and $X \in \mathcal{L}_x$, we define

$$\text{FMDD}(Y | X) = -E(\langle Y - \mu_Y, Y' - \mu_Y \rangle | X - X'),$$

where μ_Y is the mean (function) of Y and (X', Y') is an independent copy of (X, Y) .

125 To show that FMDD fully characterizes the conditional mean independence, we provide the following proposition, which is shown by using several results in Lyons (2013).

PROPOSITION 1. For $Y \in \mathcal{L}_y$, $X \in \mathcal{L}_x$, with $E(|X| + |Y|) < \infty$ and $E(|X - \mu_X||Y - \mu_Y|) < \infty$, we have

1. $\text{FMDD}(Y | X) \geq 0$;
2. $\text{FMDD}(Y | X) = 0$ if and only if H_0 is true.

130 Inspired by an unbiased estimation of MDD^2 in Park et al. (2015), we construct an unbiased estimator of FMDD by adopting the \mathcal{U} -centering approach (Székely and Rizzo, 2014; Park et al., 2015; Zhang, Yao, and Shao, 2018).

135 **DEFINITION 2.** Given iid observations $(X_i, Y_i)_{i=1}^n$ from the joint distribution of (X, Y) where X and Y can be either function-valued or vector-valued, an unbiased estimator of $\text{FMDD}(Y | X)$ is defined as

$$\text{FMDD}_n(Y | X) = \frac{1}{n(n-3)} \sum_{i \neq j} \tilde{A}_{ij} \tilde{B}_{ij}.$$

Here, $\tilde{A}_{ij}, \tilde{B}_{ij}$ are the \mathcal{U} -centered (i, j) th element of the matrices defined as

$$\tilde{A}_{ij} = \begin{cases} a_{ij} - a_{i.} - a_{.j} + a_{..} & i \neq j \\ 0 & i = j \end{cases}, \quad \tilde{B}_{ij} = \begin{cases} b_{ij} - b_{i.} - b_{.j} + b_{..} & i \neq j \\ 0 & i = j \end{cases},$$

where $a_{ij} = |X_i - X_j|$, $a_{i.} = \frac{1}{n-2} \sum_{l=1}^n a_{il}$, $a_{.j} = \frac{1}{n-2} \sum_{k=1}^n a_{kj}$ and $a_{..} = \frac{1}{(n-1)(n-2)} \sum_{k,l=1}^n a_{kl}$. In addition, $b_{ij} = \frac{1}{2}|Y_i - Y_j|^2$ and $b_{i.}, b_{.j}, b_{..}$ are defined similarly as $a_{i.}, a_{.j}, a_{..}$.

Using the same arguments presented in Appendix A.1 of Székely and Rizzo (2014) and Section 1.1 of the supplement of Zhang et al. (2018), it is not difficult to show that $\text{FMDD}_n(Y | X)$

is an unbiased estimator of $\text{FMDD}(Y | X)$ and it has the expression below.

$$\text{FMDD}_n(Y | X) = \frac{1}{\binom{n}{4}} \sum_{i < j < q < r} h(Z_i, Z_j, Z_q, Z_r),$$

where

$$h(Z_i, Z_j, Z_q, Z_r) = \frac{1}{4!} \sum_{(s,t,u,v)}^{(i,j,q,r)} (a_{st}b_{uv} + a_{st}b_{st} - a_{st}b_{su} - a_{st}b_{tv}), \quad (4)$$

with $Z_i = (X_i, Y_i)$ and $\sum_{(s,t,u,v)}^{(i,j,q,r)}$ is the summation over all permutations of the 4-tuple of indices (i, j, q, r) . For example, if $(i, j, q, r) = (1, 2, 3, 4)$, then there exist 24 permutations including $(1, 2, 3, 4), \dots, (4, 3, 2, 1)$. Then (s, t, u, v) can be any permutation of $(1, 2, 3, 4)$ and $\sum_{(s,t,u,v)}^{(1,2,3,4)}$ is the sum of all possible permutations of $(1, 2, 3, 4)$.

In the following, we state the consistency and the weak convergence of $\text{FMDD}_n(Y | X)$ as an estimator of $\text{FMDD}(Y | X)$, which are analogous to Theorems 3 and 4 in Shao and Zhang (2014).

PROPOSITION 2. *Under $E(|X| + |Y|) < \infty$ and $E(|X - \mu_X||Y - \mu_Y|) < \infty$, we have*

$$\text{FMDD}_n(Y | X) \xrightarrow{a.s.} \text{FMDD}(Y | X).$$

THEOREM 1. *Assume that $E(|X|^2 + |Y|^2) < \infty$ and $E(|X - \mu_X|^2|Y - \mu_Y|^2) < \infty$. Then under the null, we have*

$$n\text{FMDD}_n(Y | X) \xrightarrow{D} \sum_{k=1}^{\infty} \lambda_k (G_k^2 - 1),$$

where $(G_k)_{k=1}^{+\infty}$ is a sequence of iid $N(0, 1)$ random variables and $(\lambda_k)_{k=1}^{+\infty}$ is a sequence of eigenvalues corresponding to eigenfunctions $\{\psi_k(x)\}_{k=1}^{+\infty}$ such that

$$J(z, z') = \sum_{k=1}^{\infty} \lambda_k \psi_k(z) \psi_k(z')$$

where $z = (x, y)$, $J(z, z') = U(x, x')V(y, y')$, $U(x, x') = |x - x'| + E(|X - X'|) - E(|x - X'|) - E(|X - x'|)$, $V(y, y') = -\langle y - \mu_Y, y' - \mu_Y \rangle$, and (ψ_k) is an orthonormal sequence in the sense that $E\{\psi_j(Z)\psi_k(Z)\} = \mathbf{1}\{j = k\}$.

Recall that our goal is to test $H_0 : E(Y | X) = E(Y)$ almost surely which is equivalent to $\text{FMDD}(Y | X) = 0$. According to Theorem 1, it is appropriate for us to define our test statistic as

$$T_n = n\text{FMDD}_n(Y | X).$$

To understand the behavior of T_n when the null does not hold, we shall study the limiting distribution of T_n under (1) the local alternative $H_{1,n} : Y = \mu_Y + \frac{g(X)}{n^a} + \epsilon$, $a > 0$, where $g : \mathcal{L}_x \rightarrow \mathcal{L}_y$ satisfies $E\{g(X)\} = 0$, $\text{FMDD}\{g(X) | X\} > 0$ and $\epsilon \in \mathcal{L}_y$ is nondegenerate and satisfies $E(\epsilon | X) = 0$ almost surely, and $\text{pr}\{\langle g(X), \epsilon \rangle \neq 0\} > 0$; (2) the fixed alternative $H_1 : \text{FMDD}(Y | X) > 0$.

THEOREM 2. *Assume that $E\{|X|^2 + |g(X)|^2 + |\epsilon|^2\} < \infty$ and $E[|X - \mu_X|^2\{|g(X)|^2 + |\epsilon|^2\}] < \infty$. Under the local alternative $H_{1,n}$, and*

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1. if $0 < a < 1/2$,

$$T_n \xrightarrow{P} \infty;$$

2. if $a = 1/2$,

$$T_n \xrightarrow{D} c + G + \sum_{k=1}^{\infty} \lambda_k (G_k^2 - 1).$$

Here $c = \text{FMDD}\{g(X) \mid X\} > 0$ and G is a normal random variable with zero mean and variance equal to $4\text{var}\{K_1(\mathcal{Z})\}$ which is possibly correlated with $(G_k)_{k=1}^{+\infty}$, where $\mathcal{Z} = (X, \epsilon)$ and $K_1(z_1) = E\{U(x_1, X)V(\epsilon_1, g(X))\}$ with $z_1 = (x_1, \epsilon_1)$;

3. if $a > 1/2$,

$$T_n \xrightarrow{D} \sum_{k=1}^{\infty} \lambda_k (G_k^2 - 1).$$

THEOREM 3. Assume that $E(|X|^2 + |Y|^2) < \infty$ and $E(|X - \mu_X|^2 |Y - \mu_Y|^2) < \infty$. Under the alternative H_1 , we have

$$n^{1/2}\{\text{FMDD}_n(Y \mid X) - \text{FMDD}(Y \mid X)\} \xrightarrow{D} N(0, 4\sigma_1^2),$$

where $\sigma_1^2 = \text{var}\{K(Z)\}$ for $Z = (X, Y)$, and $K(z) = E\{U(x, X)V(y, Y)\}$.

Note that the limiting null distribution of our test statistic is nonpivotal in Theorem 1. Hence we use a wild bootstrap method to approximate the limiting null distribution of the test statistic and details are given in the next section.

3. BOOTSTRAP-BASED TEST

Since the limiting null distribution of our test statistic T_n is nonpivotal, we propose a wild bootstrap procedure to approximate the null distribution and show its asymptotic validity. Note that $\text{FMDD}_n(Y \mid X) = \frac{1}{n(n-3)} \sum_{i \neq j} \tilde{A}_{ij} \tilde{B}_{ij}$ is a U-statistic and its mean is zero under the null hypothesis; see (4) in Section 2. Therefore, we follow the approach of Dehling and Mikosch (1994) who proposed the weighted bootstrap for U-statistics with external random variables $(\eta_j)_{j=1}^n$. Below is the wild bootstrap procedure.

1. Generate the bootstrap statistic

$$\text{FMDD}_n^*(Y \mid X)^b = \frac{1}{n(n-3)} \sum_{i \neq j} \eta_i^{(b)} \tilde{A}_{ij} \tilde{B}_{ij} \eta_j^{(b)} \quad (5)$$

where $\eta_i^{(b)}, i = 1, \dots, n$ are iid with zero mean and unit variance, e.g., standard normal random variables.

2. Repeat step 1 for B times and collect $(T_{n,b}^*)_{b=1}^B$, where $T_{n,b}^* = n\text{FMDD}_n^*(Y \mid X)^b$.
3. Obtain the $(1 - \alpha)$ th quantile of $(T_{n,b}^*)_{b=1}^B$, $Q_{(1-\alpha),n}^*$ and set it as the critical value for the test with a significance level α .
4. Reject the null hypothesis if T_n is greater than the critical value $Q_{(1-\alpha),n}^*$ and accept H_0 otherwise.

Remark 1. Patilea et al. (2016) also proposed a wild bootstrap procedure to improve the finite sample performance of their smoothing-based test. It is worth pointing out the difference between

the two wild bootstrap procedures. In particular, Patilea et al. (2016) perturbed the response Y , i.e., $Y_i^* := \eta_i Y_i$ and computed their bootstrap test statistic based on a new bootstrap sample $(X_i, Y_i^*)_{i=1}^n$. They need to compute their bootstrapped test statistic starting from the very first step which includes dimension reduction through FPCA and finding the least favorable direction towards the null hypothesis, so their test can be computationally costly to implement. By contrast, for our wild bootstrap procedure, $(\tilde{A}_{ij}, \tilde{B}_{ij})$ only needs to be computed once and our test is simpler to implement and much faster to run than theirs.

In order to examine the asymptotic behavior of the bootstrap test statistic, we first introduce the notions of bootstrap orders and bootstrap consistency; see Remark 1 in Chang and Park (2003), Definition 2 in Li, Hsiao, and Zinn (2003).

DEFINITION 3. Let T_n^* be a bootstrap statistic that depends on the random sample $(Z_i)_{i=1}^n$. We define $T_n^* = o_p^*(1)$ a.s. if

$$pr^*(|T_n^*| > \epsilon) \rightarrow 0 \text{ a.s.},$$

for any $\epsilon > 0$, where pr^* is the conditional probability given $(Z_i)_{i=1}^n$. Moreover, we define $T_n^* = O_p^*(1)$ a.s. if for every $\epsilon > 0$, there exists a constant $M > 0$ such that for large n ,

$$pr^*(|T_n^*| > M) < \epsilon, \text{ a.s.}$$

Notice that $O_p^*(1)$ and $o_p^*(1)$ are for bootstrap sample asymptotics which have similar definition with $O_p(1)$ and $o_p(1)$. It is straightforward to extend those to $O_p^*(c_n)$ and $o_p^*(c_n)$ based on the similarity to $O_p(c_n)$ and $o_p(c_n)$, where c_n is a deterministic sequence.

DEFINITION 4. Let T_n^* be a bootstrap statistic that depends on the random sample $(Z_i)_{i=1}^n$. We say that $(T_n^* | Z_1, Z_2, \dots)$ converges to $(T | Z_1, Z_2, \dots)$ in distribution almost surely if $(T_n^* | Z_1, Z_2, \dots)$ converges to $(T | Z_1, Z_2, \dots)$ in distribution for almost every sequence (Z_1, Z_2, \dots) and the following notation is used to denote the convergence in distribution almost surely

$$T_n^* \rightarrow^{D^*} T \text{ a.s.}$$

We introduce the following theorem that is useful for deriving the asymptotic distribution of the bootstrap test statistic T_n^* .

THEOREM 4. Suppose \mathcal{H} is a symmetric kernel satisfying $E\{\mathcal{H}(Z, Z')^4\} < \infty$ and $U_n = \frac{1}{n(n-1)} \sum_{i \neq j} \mathcal{H}(Z_i, Z_j)$. Further assume that $(W_i)_{i=1}^n$ is an iid sequence of random variables with $E(W_1) = 0$, $E(W_1^2) = 1$, and $E(W_1^4) < \infty$. Then the bootstrap statistic given by $nU_n^* = \frac{1}{n-1} \sum_{i \neq j} \mathcal{H}(Z_i, Z_j) W_i W_j$, has the following asymptotic distribution.

$$nU_n^* \rightarrow^{D^*} \sum_{k=1}^{\infty} \nu_k (N_k^2 - 1) \text{ a.s.},$$

where $(N_k)_{k=1}^{+\infty}$ is a sequence of iid $N(0, 1)$ random variables and $(\nu_k)_{k=1}^{+\infty}$ is a sequence of eigenvalues associated with the kernel \mathcal{H} .

Note that the result of Theorem 4 can be viewed as an extension of Theorem 3.1 in Dehling and Mikosch (1994) to a functional data although our theoretical argument is considerably different from that in Dehling and Mikosch (1994). Based on Theorem 4, we are ready to examine the asymptotic distribution of our bootstrap statistic T_n^* under the null, local and fixed alternatives.

THEOREM 5. Assume that $E(|X|^4 + |Y|^8) < \infty$, $E(|X - \mu_X|^4 |Y - \mu_Y|^4) < \infty$ and $E(\eta^4) < \infty$. Then under the null H_0 , we have

$$T_n^* \rightarrow^{D^*} \sum_{k=1}^{\infty} \lambda_k (G_k^2 - 1) \text{ a.s.},$$

where $(\lambda_k, G_k)_{k=1}^{+\infty}$ are defined in Theorem 1.

Thus the wild bootstrap provides a consistent approximation of the limiting null distribution of our test statistic. To investigate the power of our bootstrap-based test, we derive the limit of the bootstrap test statistic under alternatives and present the results below.

THEOREM 6. Assume that $E\{|X|^4 + |g(X)|^8 + |\epsilon|^8\} < \infty$, $E(|X - \mu_X|^4 |\epsilon|^4) < \infty$ and $E(\eta^4) < \infty$. Then under the local alternative $H_{1,n}$, and

1. if $0 < a < 1/2$,

$$pr(T_n \geq Q_{(1-\alpha),n}^* | H_{1,n}) \rightarrow 1,$$

where $Q_{(1-\alpha),n}^*$ is the $(1 - \alpha)$ th quantile of the bootstrap test statistic.

2. if $a = 1/2$,

$$pr(T_n \geq Q_{(1-\alpha),n}^* | H_{1,n}) \rightarrow pr(\mathcal{G}_1 \geq Q_{(1-\alpha),\mathcal{G}_0} - c),$$

where $\mathcal{G}_1 = G + \sum_{k=1}^{\infty} \lambda_k (G_k^2 - 1)$ follows the asymptotic distribution of $T_n - c$ under $H_{1,n}$ when $a = 1/2$, and $Q_{(1-\alpha),\mathcal{G}_0}$ is the $(1 - \alpha)$ th quantile of the limiting null distribution.

3. if $a > 1/2$,

$$pr(T_n \geq Q_{(1-\alpha),n}^* | H_{1,n}) \rightarrow \alpha.$$

Under the fixed alternative H_1 with the same assumptions in Theorem 5, we have

$$pr(T_n \geq Q_{(1-\alpha),n}^* | H_1) \rightarrow 1.$$

Remark 2. Patilea et al. (2016) considered the following local alternatives $H_{1,n} : E(Y | X) = \mu_Y + r_n \delta(X)$, where r_n satisfies certain constraints which imply that $r_n n^{1/2} \rightarrow \infty$ and showed the consistency in Theorem 3.8 of their paper. By comparison, we show that our test has nontrivial power under the local alternative that approaches the null hypothesis at the rate of $n^{-1/2} = o(r_n)$ in Theorem 6, for which Patilea et al.'s (2016) test is unable to detect due to the usage of smoothing. Thus our test is more powerful than the one in Patilea et al. (2016) in terms of the capability of detecting the local alternative that approaches the null at a faster rate.

It is worth noting that the test developed by Patilea et al. (2016) has its roots from the smoothing-based tests proposed in the model specification problem; see Härdle and Mammen (1993), Fan and Li (1996), Zheng (1996), among others. The latter usually involves a consistent nonparametric estimation and thus a smoothing parameter or bandwidth is required and they are typically not sensitive to the local alternative that lies in $n^{-1/2}$ neighborhood of the null hypothesis. In the model specification testing literature, another commonly used test is of non-smoothing type, and they can be based on either an indicator function and marked empirical processes (Stute, 1997), or a characteristic function (Bierens, 1982). The non-smoothing tests typically have nontrivial power again under the local alternative of order $n^{-1/2}$, their limiting null distributions are non-pivotal, and a bootstrap-based approximation is commonly used. Our FMDD-based test is of the latter type, as the MDD has a characteristic function based definition;

see Shao and Zhang (2014). To the best of our knowledge, the advance of a non-smoothing test to the functional data setting seems new.

4. NUMERICAL SIMULATIONS

In this section, we study the finite sample performance of our FMDD-based conditional mean independence test. For convenience, we denote our test, the exponential scan test of Lei (2014), Patilea et al.'s (2016) test, and Kokoszka et al.'s (2008) test in the tables as FMDD, ES, PSS, and KMSZ, respectively. In particular, Examples 1 and 2 consider a univariate response Y and a functional covariate X , and we compare our FMDD-based test and ES test of Lei (2014). Furthermore, Example 3 studies the case of a functional response Y and a univariate covariate X , and compares with the test in Patilea et al. (2016). For the other example with a functional response Y and a functional covariate X , we compare our FMDD-based test with both PSS and KMSZ which use FPCA when constructing their test statistics. In our simulations, we set the nominal level α at 10%, 5%, 1%. For each example, the bootstrap sample size is equal to 499 and $(\eta_i)_{i=1}^n$ are from the following distribution which is same as the one used in Section 4 of Patilea et al. (2016); see Mammen (1993).

$$\eta_i = \begin{cases} \frac{-(5^{1/2}-1)}{2} & w.p. \frac{5^{1/2}+1}{2 \cdot 5^{1/2}}, \\ \frac{(5^{1/2}+1)}{2} & w.p. 1 - \frac{5^{1/2}+1}{2 \cdot 5^{1/2}}. \end{cases}$$

In order to compute the size and power of the tests, 1000 replicates are generated for all examples.

Example 1.

We consider the first example in Lei (2014). More specifically, we let $\beta_j = r\bar{\beta}_j/|\bar{\beta}|$, with $\bar{\beta}_1 = 0.3$, $\bar{\beta}_j = 4(-1)^j/j^2$ for $j \geq 2$. The covariate function X and the response variable Y are generated by

$$X_i(t) = \sum_{j=1}^{100} j^{-(1.1)/2} X_{ij} \phi_j(t), \quad Y_i = \langle X_i, \beta \rangle + \epsilon_i \quad (i = 1, \dots, n; t \in [0, 1]),$$

where X_{ij} , ϵ_i are independent standard Gaussian, $\phi_1(t) = 1$, $\phi_j(t) = 2^{1/2} \cos\{(j-1)\pi t\}$ for $j \geq 2$ and $\beta(t) = \sum_{j=1}^{100} \beta_j \phi_j(t)$. Here, r^2 corresponds to the strength of the signal and we consider $r^2 = 0, 0.1, 0.2, 0.5$, by following the simulation setting in Lei (2014). Notice that the ES test of Lei (2014) involves several user-chosen quantities. In particular, following the choices made in the code provided by Dr. Lei, we set $m_0 = 1$, $k_{n,\max} = \lceil \log_2(n^{1/3}) \rceil$, estimate the noise variance by the residual mean square in the linear regression of Y on the first $\lfloor n^{1/2} \rfloor$ estimated principal components, and use Bonferroni correction to determine the threshold value $b(m)$.

Table 1 summarizes the empirical sizes and powers of the FMDD-based test and the ES test. Both tests provide accurate empirical sizes for all cases. In terms of the power, as the strength of the signal, which is proportional to r^2 , gets stronger or sample size gets larger, the empirical powers increase for both tests. It appears that the ES test has slightly more power than our FMDD test in all cases, which is not surprising, as the ES test is tailored to the functional linear model and has certain optimality properties.

Example 2.

In this example, Y depends on X in a very nonlinear fashion as below. Let

$$Y_i = r|X_i|^2 + \epsilon_i,$$

Table 1: Percentage of rejections of the two tests for Example 1. The ES and FMDD refer to the test in Lei (2014) and the proposed test.

Size		$\alpha = 10\%$		$\alpha = 5\%$		$\alpha = 1\%$	
		$n = 50$	$n = 100$	$n = 50$	$n = 100$	$n = 50$	$n = 100$
$r^2 = 0$	FMDD	9.4	10.9	5.0	6.3	1.2	1.4
$r^2 = 0$	ES	9.6	8.8	6.0	6.0	1.4	1.4
Power		$n = 50$	$n = 100$	$n = 50$	$n = 100$	$n = 50$	$n = 100$
$r^2 = 0.1$	FMDD	27.1	43.2	15.6	30.1	4.5	11.6
$r^2 = 0.2$	FMDD	42.8	69.8	28.6	56.9	10.7	30.4
$r^2 = 0.5$	FMDD	75.6	95.3	62.9	91.4	34.0	76.2
$r^2 = 0.1$	ES	29.6	43.8	21.6	32.3	9.5	16.1
$r^2 = 0.2$	ES	47.7	70.8	36.1	61.8	20.1	41.3
$r^2 = 0.5$	ES	81.9	97.1	75.7	94.2	57.5	87.8

where X_i and ϵ_i are defined in Example 1, and $r = 0.5, 1, 2$.

From Table 2, we observe that the FMDD-based test appears superior to the ES test in terms of the empirical power in almost all cases. Note that the functional linear model assumption is not valid for this example which is presumably the main reason for the severe loss of the power for the ES test. Thus this example demonstrates the non-robustness of the ES test with respect to the model mis-specification. Our test is model free and seems preferred when it is used before constructing a particular model.

Table 2: Percentage of rejections of the two tests for Example 2. The ES and FMDD refer to the test in Lei (2014) and the proposed test.

Power		$\alpha = 10\%$		$\alpha = 5\%$		$\alpha = 1\%$	
		$n = 50$	$n = 100$	$n = 50$	$n = 100$	$n = 50$	$n = 100$
$r = 0.5$	FMDD	37.4	81.4	18.0	55.5	3.3	12.9
$r = 1$	FMDD	61.4	99.0	33.8	92.4	6.8	35.2
$r = 2$	FMDD	74.0	99.8	43.4	97.4	10.3	48.0
$r = 0.5$	ES	22.4	20.5	15.1	14.5	7.3	5.9
$r = 1$	ES	30.6	28.7	23.4	21.9	13.0	10.7
$r = 2$	ES	35.6	32.0	27.5	24.9	16.2	15.3

Example 3.

Example 3 is adopted from Patilea et al. (2016) where the data $(X_i, Y_i)_{i=1}^n$ is generated by

$$Y_i(t) = \mu(t) + \epsilon_i(t),$$

$$\mu(t) = 0.01e^{-4(t-0.3)^2},$$

where ϵ_i is an independent Brownian bridge and is independent of X_i , and X_i follows log-normal distribution with mean 3 and standard deviation 0.5. Therefore under this data generating process, X_i is independent of Y_i . In order to evaluate the power of a test, we consider the following data

generating process,

$$Y_i(t) = \mu(t)X_i + \epsilon_i(t),$$

where ϵ_i and X_i are generated in the same fashion as described above. In this example, we consider $n = 100, 200$. Recall that the test proposed by Patilea et al. (2016) involves several user-chosen parameters. Specifically when a function Y and a variable X are considered, Patilea et al.'s (2016) test requires one user-chosen parameter, i.e., the bandwidth h . Here we let $h = c_h n^{-2/9}$, $c_h = 0.75, 1.00, 1.25$ following the recommendation in Section 4.1 of Patilea et al. (2016). 310

From Table 3, the empirical sizes of both tests are reasonably close to the nominal levels. Comparing empirical sizes of the PSS tests with different values of the bandwidth parameter h , there is no uniformly best h . In other words, for different combinations of (n, α) , different values of h produce the most accurate size. For the empirical powers, our test outperforms the PSS test, which is consistent with our theory. Note that we used the R package “fdapss” available at <http://webspersoais.usc.es/persoais/cesar.sanchez/> to reproduce the test results of Patilea et al. (2016). 315

Table 3: Percentage of rejections of the two tests for Example 3. The PSS and FMDD refer to the test in Patilea et al. (2016) and the proposed test.

Size	$\alpha = 10\%$		$\alpha = 5\%$		$\alpha = 1\%$	
	$n = 100$	$n = 200$	$n = 100$	$n = 200$	$n = 100$	$n = 200$
$c_h = 0.75$ FMDD	10.8	11.6	6.1	5.9	1.4	1.2
$c_h = 0.75$ PSS	11.8	10.6	5.6	5.8	1.4	1.4
$c_h = 1.00$ PSS	12.4	10.6	5.8	5.8	1.4	0.8
$c_h = 1.25$ PSS	12.4	10.7	5.6	5.2	1.6	1.1
Power	$n = 100$	$n = 200$	$n = 100$	$n = 200$	$n = 100$	$n = 200$
$c_h = 0.75$ FMDD	83.3	98.6	74.1	97.3	48.1	86.4
$c_h = 0.75$ PSS	65.9	91.7	53.6	86.2	29.8	66.2
$c_h = 1.00$ PSS	69.7	93.5	57.2	87.5	31.9	68.9
$c_h = 1.25$ PSS	73.1	93.8	60.6	88.7	35.7	71.3

Example 4.

This example is also from Patilea et al. (2016) where both Y and X are functional data. The data is generated by the following functional linear model, 320

$$Y_i(t) = \int_0^1 \xi(s, t)X_i(s)ds + \epsilon_i(t),$$

where X_i and ϵ_i are independent Brownian Bridges, $\xi(s, t) = c \cdot \exp(t^2/2 + s^2/2)$, $c = 0, 0.75$ and we let $n = 40, 100$. Note that the PSS and the KMSZ tests require several user-chosen parameters. For the PSS test, the bandwidth parameter $h = n^{-2/9}$, the penalty value $\alpha_n = 2$, the initial guess for the direction $\gamma_0^{(q)} = (1, 1, \dots, 1)/q^{1/2} \in \mathbb{R}^q$, q is chosen as the minimum integer that explains 95% of the variance of X , and we use the sequential algorithm described in Section 3.5 in their paper with a grid size equal to 50 and these settings are the same as those 325

used in their simulation study. For the KMSZ test, p and q are chosen by the minimum values which explain at least 95% of variances of Y and X , respectively.

According to Table 4, our FMDD-based test is superior to the other two tests with respect to the empirical size and power. In particular, size performances of all three tests are comparable with the KMSZ test showing slight conservativeness in size. Under the alternatives, all three tests deliver nontrivial powers where our test always has the highest power, especially for $n = 40$. Notice that Y follows the functional linear model for this example and therefore the KMSZ test is expected to perform well since the KMSZ test is tailored to the functional linear model. It is interesting that the FMDD-based test performs better than the KMSZ test indicating that projecting the functional data to a finite dimensional space could lead to some loss of power, especially when the sample size is small.

Table 4: Percentage of rejections of the three tests for Example 4. The PSS, KMSZ, and FMDD refer to the test in Patilea et al. (2016), the test in Kokoszka et al. (2008), and the proposed test, respectively.

Size	$\alpha = 10\%$		$\alpha = 5\%$		$\alpha = 1\%$	
	$n = 40$	$n = 100$	$n = 40$	$n = 100$	$n = 40$	$n = 100$
FMDD	11.0	10.6	5.7	4.7	1.4	1.3
PSS	9.1	10.9	5.3	5.5	1.2	1.7
KMSZ	9.3	9.0	3.5	4.2	0.3	0.7
Power	$n = 40$	$n = 100$	$n = 40$	$n = 100$	$n = 40$	$n = 100$
FMDD	99.6	100.0	99.5	100.0	95.2	100.0
PSS	77.8	99.7	67.7	99.4	42.3	97.7
KMSZ	97.7	100.0	90.4	100.0	57.6	100.0

From the previous four simulation examples, we observe that our FMDD test has an accurate size at all nominal levels, which means the wild bootstrap does an excellent job of approximating the finite sample distribution of our test statistic under the null. Our test shows comparable or higher power in all examples, as compared to the ES, the KMSZ and the PSS tests. An appealing feature of our FMDD test is that there is no tuning parameter involved and the validity of our test does not rely on a linear model assumption. A possible explanation for the power advantage of the FMDD test in comparison with the KMSZ and the PSS tests is that both KMSZ and PSS tests use FPCA to reduce the functional data to finite dimension while our test statistic is constructed by preserving the functional form of the data. Some loss of power might occur due to the use of a dimension reduction device when computing a test statistic.

5. DATA ILLUSTRATION

In this section, we consider Tecator dataset and it is available in the `fda.usc` package in R. The dataset contains 215 meat samples, consisting of a 100-channel spectrum of absorbances measured along the discretized points of the wavelength range 850-1050nm and the contents of water, fat, and protein, measured in percent. Tecator dataset has been considered in the literature of functional data analysis; see García-Portugués, González-Manteiga, and Febrero-Bande (2014), Ferraty and Vieu (2006, Chapter 2, 7, 9), Aneiros-Pérez and Vieu (2006), Rossi et al. (2005) among others. Following the aforementioned articles, we are interested in modeling the

percentage of fat Y as the response and study its relationship with the spectrometric curves, X ; see Figure 1.

Since the response variable is a scalar and the predictor variable is function-valued, we apply our method and the ES test of Lei (2014) in order to test the conditional mean independence. More precisely, the bootstrap sample size is 500 for our test and the user-chosen parameters in Lei (2014) are set the same as those described in Example 2. Our FMDD-based and the ES test easily reject the null hypothesis under $\alpha = 10\%$, 5% , 1% which indicates that the predictor variable significantly contributes to the conditional mean of Y .

To make the testing problem more realistic, we remove the linear effect of X on Y and test the conditional mean independence of the residual/error part ϵ on the covariate X , by applying our FMDD-based test with the wild bootstrap method. Specifically let

$$Y = \beta_0 + \langle X, \beta \rangle + \epsilon, \quad (6)$$

where β_0 is an intercept, $\beta(\cdot)$ is a slope function and ϵ is the error. We test

$$H_0 : E(\epsilon | X) = 0 \text{ almost surely} \quad \text{versus} \quad H_1 : \text{pr}\{E(\epsilon | X) \neq 0\} > 0. \quad (7)$$

We compute our test statistic as

$$T_n = n\text{FMDD}_n(\hat{\epsilon} | X) \quad (8)$$

where $\hat{\epsilon} = Y - \hat{\beta}_0 - \langle X, \hat{\beta} \rangle$ is the residual and $\hat{\beta}_0$, $\hat{\beta}(\cdot)$ are the estimates of the intercept and slope function. Assume that $\hat{\beta}(t) = \sum_{k=1}^d \hat{\beta}_k \phi_k(t)$ with $(\phi_k)_{k=1}^d$ being a sequence of basis functions and $(\hat{\beta}_k)_{k=1}^d$ being the estimated coefficients. We estimate the limiting null distribution of our test statistic by using the wild bootstrap method described below.

1. Let $\eta_i^{(b)}$ be iid random variables with zero mean and unit variance. Compute the wild bootstrap statistic

$$\begin{aligned} n\text{FMDD}_n^*(\hat{\epsilon} | X)^b &= \frac{1}{(n-3)} \sum_{i \neq j} \eta_i^{(b)} \tilde{A}_{ij} \tilde{B}_{ij} \eta_j^{(b)} \\ &+ \frac{1}{n} \left\{ \sum_{i=1}^n (X_i - \bar{X}) \hat{\epsilon}_i \eta_i^{(b)} \right\}^T Q_n \frac{1}{n(n-3)} \sum_{k \neq l} \tilde{S}_{kl} \tilde{A}_{kl} Q_n \left\{ \sum_{j=1}^n (X_j - \bar{X}) \hat{\epsilon}_j \eta_j^{(b)} \right\} \\ &- \frac{2}{(n-3)} \left\{ \sum_{i=1}^n (X_i - \bar{X}) \hat{\epsilon}_i \eta_i^{(b)} \right\}^T Q_n \sum_{j=1}^n \left\{ \frac{-1}{n} \sum_{i \neq j} \hat{\epsilon}_j (X_i - \bar{X}) \tilde{A}_{ij} \right\} \eta_j^{(b)}, \end{aligned}$$

where \tilde{A}_{ij} and \tilde{B}_{ij} are calculated based on $(\hat{\epsilon}_j, X_j)_{j=1}^n$, $S_{ij} = \frac{1}{2}(C_i - C_j)(C_i - C_j)^T$ with $C_i = (\langle X_i, \phi_1 \rangle, \dots, \langle X_i, \phi_d \rangle)^T$, \tilde{S}_{ij} is the \mathcal{U} -centered version of S_{ij} , and $Q_n^{-1} = \frac{1}{n} \sum_{i=1}^n (C_i - \bar{C})(C_i - \bar{C})^T$ with $\bar{C} = \frac{1}{n} \sum_{i=1}^n C_i$.

2. Repeat step 1 for B times and collect $(T_{n,b}^*)_{b=1}^B$, where $T_{n,b}^* = n\text{FMDD}_n^*(\hat{\epsilon} | X)^b$.
3. Calculate the empirical p-value as $\frac{1}{B} \sum_{b=1}^B \mathbf{1}\{T_{n,b}^* > T_n\}$.

Here the bootstrap statistic is more complicated than the one in Section 3. However, the bootstrap statistic above is derived after considering the estimation effect caused by replacing unknown ϵ by $\hat{\epsilon}$ which appears in the limiting null distribution of T_n in (8). With the aid of the wild bootstrap, the estimation effect is hopefully captured and a rigorous theoretical justification is currently being investigated and will be reported in another paper.

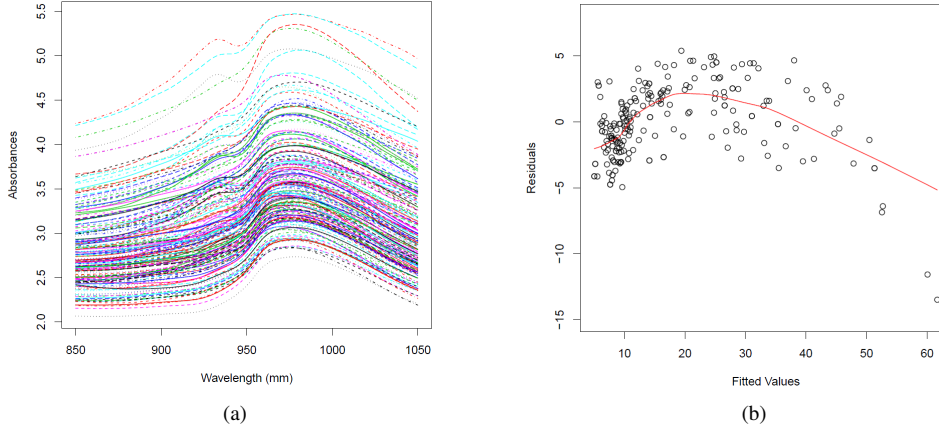


Fig. 1: Predictor functions and the residual plot. (a) Plot of predictor functions. (b) Residual plot obtained after fitting the functional linear model in (6).

390 To illustrate the usefulness of our FMDD test and the associated wild bootstrap procedure, we test (7). This is equivalent to the diagnostic checking for the functional linear model; see Section 6 for more discussions. In particular, we fit the functional linear model to (Y, X) by using the function `fregre.basis` in the `fda.usc` package where the basis functions are the cubic splines which are chosen by default from the function `fregre.basis` and use the residual to
 395 test the conditional mean independence in H_0 . The ES test has p-values equal to 1.000 1.000 0.907 with respect to $k = 1, \dots, k_{n,\max}$ for $k_{n,\max} = 3$. Hence, the ES test indicates that there are no significant evidence to reject the null hypothesis under the assumption that ϵ and covariate follow the functional linear model. However, the p-value of our FMDD-based test is 0.000 which strongly suggests that the functional linear model is not sufficient for describing the conditional
 400 distribution of Y given X . We further generate the residual plot, residuals versus fitted values; see Figure 1. The figure supports the test result of the FMDD and suggests that X can be nonlinearly dependent with Y .

6. DISCUSSION AND CONCLUSIONS

To conclude, we mention two related future research topics. On one hand, the diagnostic
 405 checking for the functional linear model is worth investigating given the prevalence of the functional linear model in practical applications. As we discussed in Section 5, the estimation effect from replacing $\epsilon = Y - \beta_0 - \langle X, \beta \rangle$ by the residual $\hat{\epsilon}$ is expected to show up in the limiting null distribution, and it seems that the proposed wild bootstrap in Section 5 can capture the estimation effect and be consistent. A careful theoretical investigation is needed. On the other
 410 hand, it would be interesting to extend the idea to test for the conditional quantile independence owing to a natural connection between conditional quantile independence and conditional mean independence when the response Y is a scalar-valued variable; see Shao and Zhang (2014). Also see Kato (2012) for estimation in the functional linear quantile regression when the response Y is a scalar random variable. When Y is function-valued, Chowdhury and Chaudhuri (2016)
 415 recently advanced nonparametric quantile regression to a functional data based on spatial depth and quantiles. It would be intriguing to see how the FMDD can play a role in the model checking and the testing for nonparametric quantile regression models.

ACKNOWLEDGEMENT

Both Zhang and Shao's research are partially supported by NSF grants. Chung Eun Lee and Xianyang Zhang equally contribute to this paper, and the authors are listed in the alphabetical order. We would like to thank Dr. Jing Lei for providing the R code used in Lei (2014), and the editor and two referees for thoughtful comments that led to a substantial improvement of the paper.

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