# Multivariate Functional Halfspace Depth

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October 10, 2013

A depth for multivariate functional data is defined and studied. By the multivariate nature and by including a weight function, it acknowledges important characteristics of functional data, namely differences in the amount of local amplitude, shape and phase variation. Both population and finite sample versions are studied. The multivariate sample of curves may include warping functions, derivatives and integrals of the original curves for a better overall representation of the functional data via the depth. A simulation study and data examples confirm the good performance of this depth function.

Keywords: statistical depth, functional data, time warping, multivariate data.

Nowadays, functional data are frequently observed and many statistical methods

#### 1 Introduction

have been developed to retrieve useful information from these data sets. Typically, the observed data consist of a set of N curves, each measured at different time points  $\overline{\phantom{a}}^1$ Gerda Claeskens is Professor, ORSTAT, KU Leuven, Naamsestraat 69, 3000 Leuven, Belgium (E-mail: Gerda. Claeskens@kuleuven.be. Mia Hubert is Professor, Department of Mathematics, KU Leuven, Celestijnenlaan 200B, 3001 Leuven, Belgium (E-mail: Mia. Hubert@wis. kuleuven.be). Leen Slaets is now Statistician at EORTC, Brussels, Belgium, part of this research was performed during her doctoral studies at ORSTAT. Kaveh Vakili is a doctoral student at the Department of Mathematics, KU Leuven, Celestijnenlaan 200B, 3001 Leuven, Belgium (E-mail: Kaveh. Vakili@wis. kuleuven.be). All authors are affiliated with the Leuven Statistics Research Center and acknowledge the support of KU Leuven grant GOA/12/14 and of the IAP Research Network P7/06 of the Belgian Science Policy. The authors thank B. De Ketelaere for providing the data, and the reviewers for their comments.

 $t_1, \ldots, t_T$ . For an overview, see Ramsay and Silverman (2006); Ferraty and Vieu (2006). Basic questions of interest in functional data analysis (FDA) are (i) the estimation of the central tendency of the curves, (ii) the estimation of the variability among the curves, (iii) the detection of outlying curves, as well as (iv) classification and clustering of such curves.

In this paper we consider multivariate functional data. We observe for all observation units at each time point a K-dimensional vector of measurements, which arise from an underlying set of K curves. A popular example is the bivariate gait data set, which contains the simultaneous variation of the hip and knee angles for 39 children at 20 equally spaced time points (Ramsay and Silverman, 2006). Berrendero et al. (2011) have K = 3 when recording daily temperature functions at 3, 9 and 12cm below the surface during N = 21 days. Sangalli et al. (2009) and Pigoli and Sangalli (2012) present several multivariate functional data from medical studies. Bivariate weather data are studied in Section 3.2.

Different types of multivariate functional data arise by computing additional curves, starting from one observed set of univariate functional data. A well-studied situation is the addition of the first order derivatives which provides additional information on the shape of the curves and consequently is interesting to detect curves with an outlying shape (Cuevas et al., 2007). Note that this is different from a common practice in chemometrics, where observed spectral data are often replaced by their first-order derivatives in order to eliminate baseline features. Also higher order derivatives could be added. This has been applied in the Berkeley growth data set (Ramsay and Silverman, 2006), which contains the heights of children and the estimated acceleration curves that correspond to the second-order derivatives.

In this paper we introduce to the depth calculation the inclusion of other functions of the original set of curves (such as warping functions, derivatives, integrals,...)

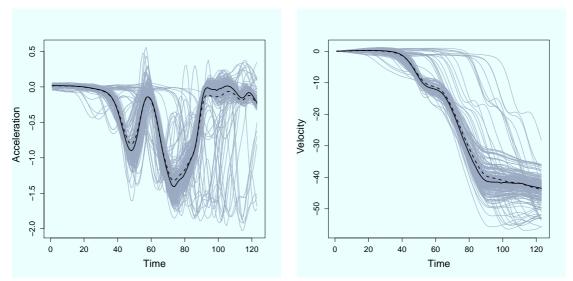


Figure 1: Industrial data: (a) Acceleration and (b) velocity signals, with cross-sectional mean curve (dashed line) and depth-based median curve (solid black line).

which allows us to obtain more powerful conclusions about the data-driven process. Some interesting functions are obtained from a warping procedure, which often precedes the analysis of functional data. Typically some warping method (also known as curve alignment) is applied to the observed curves as a preprocessing step, but no further information is retained from this analysis. In Slaets et al. (2012) it is shown how the information from the warping procedure can be incorporated into a clustering method for functional data. In Section 4.3 we show the benefits of a multivariate analysis of the warped data together with the curves obtained via the warping function.

A different augmentation of the data is presented in Section 3. It contains the analysis of a real data set which consists of acceleration signals over time from an industrial machine (De Ketelaere et al., 2011). Most of the observed curves, see Figure 1(a), follow a similar nonlinear pattern, but we also notice several curves with a deviating trend, most prominently at the final stage of the production. In addition to these acceleration signals, we do not use their derivatives but rather the

integrated curves as they represent the underlying velocity, see Figure 1(b). Also here, we observe a global structure as well as deviating signals. On both plots we have added the cross-sectional mean curve (dashed line). Further we have plotted our new estimator for the central tendency of the curves, shown as a solid black line. It is already obvious that these estimates are less influenced by the outlying curves. For the velocity curves, the effect is less pronounced as the outlying curves occur in both directions of the central pattern.

Our approach to estimate the central tendency of multivariate functional data is based on the concept of depth. Depth functions were initially defined for multivariate data. They provide an ordering from the center outwards such that the most central object gets the highest depth value and the least central objects the smallest depth. More recently, several notions of depth have been proposed for univariate functional data, such as the integrated depth (ID, Fraiman and Muniz, 2001), the h-mode and random projection depth (RP, Cuevas et al., 2007), the band depth and modified band depth (MBD, López-Pintado and Romo, 2009) and the half-region depth (López-Pintado and Romo, 2011). The ID depth and MBD depth are quite similar, as they both consider a (univariate) depth function at each time point t and define the functional depth as the average of these depth values over all time points. Cuevas et al. (2007) have proposed to consider the curves and their derivatives, yielding the bivariate random projection depth (RPD). For a number of random projections, they project both sets of curves on each direction, apply a multivariate depth function on the bivariate sample and finally average the depth values over the random projections.

We generalize several of these ideas by constructing a depth function for K-variate samples of curves, which we define the multivariate functional depth (MFD). Our definition averages a multivariate depth function over the time points, but in addition it includes a weight function. This weight function can be chosen as to account

for variability in amplitude, to adapt to the functional nature of the data. More specifically we choose Tukey's halfspace depth (Tukey, 1975) as the building block, which leads to the multivariate functional halfspace depth (MFHD).

The population and finite-sample definition of MFD and MFHD and their main properties are given in Section 2. We define and characterize the MFD median, as the curve with maximal MFD. In Section 3 we illustrate using two data sets how this new depth concept can be used to estimate the central tendency of the curves, as well as the variability among the curves. In Section 4 we provide the results of a simulation study in which we compare several depth functions and several augmented data sets (such as by including derivatives and warping functions). Section 5 concludes and gives directions for further research. All proofs are collected in the Appendix. The supplementary material illustrates on the industrial data set the effect of adding the velocity curves to the analysis.

# 2 Definition and properties of multivariate functional depth

### 2.1 Notation

Consider a K-variate (finite K), real-valued stochastic process of continuous functions  $\mathbf{\mathcal{Y}} = (\mathcal{Y}_1, \dots, \mathcal{Y}_K)$  with for  $j = 1, \dots, K$ ,  $\mathcal{Y}_j : U \to \mathbb{R} : t \mapsto \mathcal{Y}_j(t)$  continuous on a compact interval U and denote its cumulative distribution by  $F_{\mathbf{\mathcal{Y}}}$ . Thus, for every finite set of time points  $t_1, \dots, t_T \in U$ ,  $(\mathbf{\mathcal{Y}}(t_1), \dots, \mathbf{\mathcal{Y}}(t_T))$  is a random variable on  $(\mathbb{R}^K)^T$  and at each time point  $t \in U$ ,  $\mathbf{\mathcal{Y}}(t)$  is a K-variate random variable with associated cumulative distribution function (cdf)  $F_{\mathbf{\mathcal{Y}}(t)}$ .

Real numbers, vectors, continuous functions on an interval U and vectors of functions are all used in conjunction with each other. To avoid confusion, we provide an overview of the notation that is used throughout this paper. The set of continuous functions on U is denoted by  $\mathcal{C}(U)$ . Elements thereof and their graphs are denoted by capital letters (e.g. X). For K-vectors of continuous functions in  $\mathcal{C}(U)^K$  and their graphs, bold capital letters are used (e.g. X) or the vector notation  $(X_1, \ldots, X_K)$  where  $X_i \in \mathcal{C}(U)$ . The function value of a curve X at a time point t is denoted by  $X(t) \in \mathbb{R}$ . The vector of function values of an element X in  $\mathcal{C}(U)^K$  at a time point t is denoted by  $X(t) = (X_1(t), \ldots, X_K(t))$ . The empirical cumulative distribution function based on a sample  $\{Y_1(t), \ldots, Y_N(t)\}$  each with the same distribution as  $\mathcal{Y}(t)$  is denoted by  $F_{\mathcal{Y}(t),N}$ . For vectors in  $\mathbb{R}^K$ , bold lowercase letters are used (e.g. a) or the vector notation  $(a_1, \ldots, a_K) \in \mathbb{R}^K$ . For matrices capital letters early in the alphabet are used (e.g. A), while later letters (e.g. X) are reserved for curves. For real numbers, lowercase letters are used (e.g. a).

#### 2.2 Population definition

#### 2.2.1 A general multivariate depth as building block

A depth function provides an ordering from the center outwards such that the most central objects get the highest depth and the least central objects the smallest depth. Let  $D(\cdot; F_{\mathcal{X}}) : \mathbb{R}^K \to [0, 1]$  be a statistical depth function for the probability distribution of a K-variate random vector  $\mathcal{X}$  with cdf  $F_{\mathcal{X}}$ , according to Zuo and Serfling (2000a). Associated with the depth function is the depth region  $D_{\alpha}(F_{\mathcal{X}})$  at level  $\alpha \geqslant 0$ , defined as  $D_{\alpha}(F_{\mathcal{X}}) = \{x \in \mathbb{R}^K : D(x; F_{\mathcal{X}}) \geqslant \alpha\}$ .

The new definition of multivariate functional depth combines the local depths of  $\mathbf{y}(t)$  at each time point  $t \in U$  and includes a weight function that may be specified for different purposes.

**Definition 1.** Consider a K-variate stochastic process  $\{\mathbf{y}(t), t \in U\}$  on  $\mathbb{R}^K$  with cdf  $F_{\mathbf{y}}$  that generates continuous paths in  $C(U)^K$ . Let D be a statistical depth function on  $\mathbb{R}^K$  and w a weight function that is defined on U and integrates to one. Take an

arbitrary  $\mathbf{X} \in \mathcal{C}(U)^K$ . The multivariate functional depth (MFD) of  $\mathbf{X}$  is defined as

$$MFD(\boldsymbol{X}; F_{\boldsymbol{\mathcal{Y}}}) = \int_{U} D(\boldsymbol{X}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) \cdot w(t) dt.$$
 (1)

This weight function may or may not depend on  $F_{\mathbf{y}(t)}$ ,  $t \in U$ . A first example for the weight is a constant times an indicator for a range of interest. This allows for example to eliminate the effect of a start-up phase in an industrial process, or to remove imprecise measurements during certain regions which often happens for spectral data. A second example takes the local changes in the amount of variability in amplitude (vertical variability) into account by defining

$$w(t) = w_{\alpha}(t; F_{\mathbf{y}(t)}) = \operatorname{vol}\{D_{\alpha}(F_{\mathbf{y}(t)})\} / \int_{U} \operatorname{vol}\{D_{\alpha}(F_{\mathbf{y}(u)})\} du, \tag{2}$$

which is proportional to the volume of the depth region at time point t. This implies that for regions where all curves nearly coincide the weight is small, heuristically, the order of the curves does not matter much here. For regions where the amplitude variability is large, there is a visual ordering of the curves, and the influence of those regions on the functional depth will be large. See Section 3.1 for an illustration. When the weight function (2) is considered, we denote the corresponding depth by  $MFD(\alpha)$ . Note that for many cases the definition of MFD with this choice of weight does not depend on  $\alpha$ . In general, the value of  $\alpha$  is irrelevant when at each time point t the volumes of the depth regions are proportional to a fixed function of  $\alpha$ . In particular, for most depth functions, it holds that at unimodal elliptic symmetric distributions, the contours of the depth regions coincide with density contours (Zuo and Serfling, 2000b). This implies that the choice of  $\alpha$  in MFD( $\alpha$ ) becomes irrelevant (at least at the population level) when the elliptic distributions remain the same for all t up to a scale change. Also the opposite approach could be considered, in which the weight is large in regions where all curves nearly coincide, in order to strongly penalize outlying curves in these time intervals.

In Theorem 1 we show that the multivariate functional depth satisfies some key properties, adapted to a functional data context, that were put forward by Zuo and Serfling (2000a). All proofs are relegated to the Appendix.

**Theorem 1.** Assume that the depth function D satisfies the four properties listed in Zuo and Serfling (2000a), i.e. affine invariant, maximal at the center, monotone relative to the deepest point and vanishing at infinity. Then MFD, as defined in Definition 1, is a statistical depth function satisfying the following key properties:

(i) Affine invariance (invariance w.r.t. the underlying coordinate system). If the weight function w is affine invariant, then

$$MFD(\boldsymbol{X}; F_{\boldsymbol{y}}) = MFD(\boldsymbol{A}\boldsymbol{X}_{(ct+d)} + \tilde{\boldsymbol{X}}_{(ct+d)}; F_{\boldsymbol{A}\boldsymbol{y}_{(ct+d)} + \tilde{\boldsymbol{X}}_{(ct+d)}}),$$

with U = [l, u],  $\mathbf{A}\mathbf{Y}_{(ct+d)} + \tilde{\mathbf{X}}_{(ct+d)}$  the stochastic process  $\{\mathbf{A}\mathbf{Y}(\frac{s-d}{c}) + \tilde{\mathbf{X}}(\frac{s-d}{c}), s \in S = [cl+d, cu+d]\}$  for any constants  $c \in \mathbb{R}_0$ ,  $d \in \mathbb{R}$ , any vector of functions  $\tilde{\mathbf{X}} \in \mathcal{C}(U)^K$  and any matrix  $\mathbf{A} \in \mathbb{R}^{K \times K}$  with  $\det(\mathbf{A}) \neq 0$ , and  $\tilde{\mathbf{X}}_{(ct+d)}$  the curve  $\{s, \tilde{\mathbf{X}}(\frac{s-d}{c})\}$ , with  $s \in S = [cl+d, cu+d]$ .

- (ii) Maximality at the center. For a uniquely defined  $\Theta \in \mathcal{C}(U)^K$  such that  $\Theta(t)$  is a symmetry point in which D is maximal at every  $t \in U$ , it holds that  $MFD(\Theta; F_{\mathcal{Y}}) = \sup_{\mathbf{X} \in \mathcal{C}(U)^K} MFD(\mathbf{X}; F_{\mathcal{Y}})$ .
- (iii) Monotonicity relative to the deepest point. Let  $\Theta \in \mathcal{C}(U)^K$  such that  $\Theta(t)$  is a deepest point at every  $t \in U$ , then for any  $a \in [0,1]$ ,  $MFD(\boldsymbol{X}; F_{\boldsymbol{\mathcal{Y}}}) \leqslant MFD(\boldsymbol{\Theta} + a(\boldsymbol{X} \boldsymbol{\Theta}); F_{\boldsymbol{\mathcal{Y}}})$ .
- (iv) Vanishing at infinity. For  $1 \leq k \leq K$  and for a series of curves  $X_{n,k}$  with  $\lim_{n\to\infty} |X_{n,k}(t)| = \infty$  for almost all time points t in U:  $\lim_{n\to\infty} MFD(X_{n,k}; F_{\mathbf{y}}) = 0$ .

The affine invariance holds for all specified weight functions. When the weight is invariant with respect to transformations  $t \mapsto A(t)X(t) + \tilde{X}(t)$ , the same holds for MFD. In the original multivariate setting, the fourth property, 'vanishing at infinity',

requires that for a vector  $\boldsymbol{x} \in \mathbb{R}^K$  the depth of  $\boldsymbol{x}$  should converge to 0 for  $\|\boldsymbol{x}\| \to \infty$ . When a curve behaves in accordance with the sample on the majority of the interval and, e.g., converges to infinity near the border, one might not wish to attribute zero depth. The vanishing at infinity property for functional depth holds as stated in (iv). See also López-Pintado and Romo (2009, p. 725- for -726) and Nieto-Reyes (2011).

Theorem 2 states the existence of a deepest MFD curve. As a result an MFD median can be defined, see Definition 2. We use a generalized maximum theorem (Ausubel and Deneckere, 1993) to obtain continuity related properties of the maximum depth function and of the deepest values, the arg-max correspondence (i.e. set-valued function)  $\Theta$ .

Define the function  $\mathcal{H}: U \times \mathbb{R}^K \to [0,1]: (t,\boldsymbol{x}) \mapsto \mathrm{D}(\boldsymbol{x},F_{\boldsymbol{\mathcal{Y}}(t)}) = \mathcal{H}(t,\boldsymbol{x})$ . Define  $\gamma: U \to \mathbb{R}^K$  a correspondence that is non-empty and compact-valued. In particular  $\gamma(t)$  specifies for every t the set of  $\boldsymbol{x} \in \mathbb{R}^K$  for which we would be interested in computing the depth. Since the process  $\boldsymbol{\mathcal{Y}}(t)$  is continuous, its range is compact, a compact set enclosing the range of  $\boldsymbol{\mathcal{Y}}(t)$  will satisfy the purpose, it may be the same one for all  $t \in U$ . Define  $\Pi: U \to \mathbb{R}: t \mapsto \Pi(t) = (-\infty, \max_{\boldsymbol{x} \in \gamma(t)} D(\boldsymbol{x}; F_{\boldsymbol{\mathcal{Y}}(t)})]$ . Denote by  $G(t) = \{(x, \mathcal{H}(t, \boldsymbol{x})); \boldsymbol{x} \in \gamma(t)\}$  the graph of  $\mathcal{H}(t, \cdot)$  restricted to  $\gamma(t)$ , for  $t \in U$ , and by  $\overline{G}(t)$  its closure in  $\mathbb{R}^K \times \mathbb{R} \cup \{-\infty\}$ . Define the correspondence  $\widetilde{G}: U \to \mathbb{R}^K \times \mathbb{R} \cup \{-\infty\}$  with

$$\widetilde{G}(t) = \{(\boldsymbol{x}, y) : \text{ there exist } y', y'' \in \mathbb{R} \cup \{-\infty\} \text{ such that } y'' \leq y \leq y',$$

$$(\boldsymbol{x}, y') \in \overline{G}(t) \text{ and } (\boldsymbol{x}, y'') \in \overline{G}(t)\}.$$

**Theorem 2.** Assume either set of conditions (a) or (b).

(a) The function  $\mathcal{H}$  is upper-semicontinuous,  $\gamma$  is an upper-hemicontinuous correspondence that is non-empty and compact-valued, and  $\Pi$  is a lower-hemicontinuous correspondence.

(b) The function  $\mathcal{H}$  is an upper-semicontinuous function of  $\mathbf{x}$  for every  $t \in U$ ,  $\gamma$  is a correspondence that is non-empty and compact-valued, and  $\widetilde{G}$  is a continuous correspondence.

Then,

- (i) The maximum depth function  $U \to [0,1] : t \mapsto \max_{\boldsymbol{x} \in \gamma(t)} D(\boldsymbol{x}; F_{\boldsymbol{y}(t)})$  is continuous.
- (ii) Concerning the values where maximum depth is reached,

$$\Theta: U \to \mathbb{R}^K: t \mapsto \arg \max_{\boldsymbol{x} \in \gamma(t)} D(\boldsymbol{x}; F_{\boldsymbol{y}(t)})$$

is a non-empty, compact-valued and upper-hemicontinuous correspondence. If  $\Theta$  is single-valued, it is continuous.

(iii) Consider a curve  $\boldsymbol{\vartheta}$  for which at each time point t,  $\boldsymbol{\vartheta}(t) \in \boldsymbol{\Theta}(t)$ . Then, if  $t \mapsto D(\boldsymbol{\vartheta}(t); F_{\boldsymbol{\mathcal{Y}}(t)})w(t)$  is measurable, il holds for all  $\boldsymbol{X} \in \mathcal{C}(U)^K$ ,

$$MFD(\boldsymbol{X}; F_{\boldsymbol{\mathcal{Y}}}) \leqslant \int_{U} D(\boldsymbol{\vartheta}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) \cdot w(t) \ dt.$$

If moreover  $\boldsymbol{\vartheta} \in \mathcal{C}(U)^K$ , then  $MFD(\boldsymbol{\vartheta})$  is maximal.

(iv) Any curve  $\vartheta \in \mathcal{C}(U)^K$  with maximal MFD should have maximal depth D at each time point t, i.e.  $\vartheta(t) \in \Theta(t)$ .

Note that if  $\Theta$  is single-valued and  $\mathcal{H}$  is continuous, the continuity of  $\Theta$  follows directly from Berge's maximum theorem (e.g. Abalo and Kostreva, 2005, Cor. 1).

**Definition 2.** Assume the conditions of Theorem 2 and that  $\Theta$  is single-valued. We then define  $M_{MFD}(\mathcal{Y}) = \Theta$  the MFD median of  $\mathcal{Y}$ .

The MFD median is affine equivariant, following the definitions in Theorem 1(i), i.e.  $M_{\text{MFD}}(A\boldsymbol{\mathcal{Y}}_{(ct+d)} + \tilde{\boldsymbol{X}}_{(ct+d)}) = \boldsymbol{A} \ M_{\text{MFD}}(\boldsymbol{\mathcal{Y}}) + \tilde{\boldsymbol{X}}_{(ct+d)}$ . This property is not satisfied by the cross-sectional median. Moreover it does not depend on the weight

function. Consequently, unlike the depth values and the central regions, the MFD median based on MFD( $\alpha$ ) does not depend on  $\alpha$ . Note too that the MFD median is in general not one of the observed curves.

#### 2.2.2 Halfspace depth as a building block

In the remainder of the paper we mainly focus on halfspace depth (Tukey, 1975). For  $\mathcal{X}$  a random variable on  $\mathbb{R}^K$  with cumulative distribution function  $F_{\mathcal{X}}$  and a vector  $\mathbf{x} \in \mathbb{R}^K$  the population halfspace depth (Tukey depth) is defined as

$$HD(\boldsymbol{x}; F_{\boldsymbol{\mathcal{X}}}) = \inf_{\boldsymbol{u} \in \mathbb{R}^K, ||\boldsymbol{u}||=1} P(\boldsymbol{u}'\boldsymbol{\mathcal{X}} \geqslant \boldsymbol{u}'\boldsymbol{x}).$$
(3)

The resulting MFD depth is called the multivariate functional halfspace depth (MFHD). The notation MFHD( $\alpha$ ) is used when the weight function (2) is considered. It is well known that the halfspace depth regions are compact convex subsets of  $\mathbb{R}^K$  (Rousseeuw and Ruts, 1999). Theorem 2 of Mizera and Volauf (2002) then guarantees through the upper-hemicontinuity of the depth regions and the compactness of U, together with the closedness and boundedness of the depth regions that the weight function (2) is well defined. For a practical choice of  $\alpha$ , see Section 2.3.2. We also choose HD because it satisfies the requirements of a building block for the functional depth as stated in Theorem 1. Consequently MFHD is affine invariant, maximal at the point (curve) of symmetry, monotone relative to the deepest point, and vanishing at infinity. An additional advantage of HD is its robustness with respect to outliers. The influence function of the HD of any multivariate point in  $\mathbb{R}^{K}$  is bounded (Romanazzi, 2001) and the deepest point (Tukey median) has a positive breakdown value between 1/(K+1)and 1/3 at absolutely continuous distributions (Chen and Tyler, 2002). Finally, fast algorithms exist for the computation of HD at multivariate data, as well as for the depth regions and for the Tukey median (see Section 2.3 for details).

Let the curve  $\Theta$  be defined as in Theorem 2, i.e.  $\Theta(t)$  contains the set of vectors in

 $\mathbb{R}^K$  with maximum value of  $\mathrm{HD}(\cdot; F_{\mathcal{Y}(t)})$ . If  $\Theta$  is single-valued, we call it the MFHD median of  $\mathcal{Y}$ , similar to Definition 2. When uniqueness of the deepest point at each time point is not assumed, we can define  $M_{\mathrm{MFHD}}(\mathcal{Y})$  as the curve which equals at each time point t the center of mass of  $\Theta(t)$ . Under the conditions of Theorem 2 we obtain the upper-hemicontinuity of  $\Theta$ . It might be possible to find conditions that guarantee that taking the center of mass of  $\Theta(t)$  is continuous as a function of  $t \in U$ , however, this would lead too far for the present purpose.

#### 2.3 Finite sample definition

#### 2.3.1 A general multivariate depth as a building block

In practice one does not observe curves, but rather curve evaluations at a set of time points  $t_1 < t_2 < \ldots < t_T$  in  $U = [t_1, t_T]$ , not necessarily equidistant.

**Definition 3.** For a sample of multivariate curve observations  $\{ \mathbf{Y}_1(t_j), \dots, \mathbf{Y}_N(t_j); j = 1, \dots, T \}$ , with at each time point t cdf  $F_{\mathbf{y}(t),N}$ , the sample multivariate functional depth at  $\mathbf{X} \in \mathcal{C}(U)^K$  is defined by, with  $t_0 = t_1$ ,  $t_{T+1} = t_T$  and  $W_j = \int_{(t_{j-1}+t_j)/2}^{(t_j+t_{j+1})/2} w(t) dt$ ,

$$MFD_N(\boldsymbol{X}) = \sum_{j=1}^T D(\boldsymbol{X}(t_j); F_{\boldsymbol{y}(t_j),N}) W_j.$$
(4)

Special cases. For a constant weight w(t) = w for all  $t \in U$ ,  $W_j = w \cdot (t_{j+1} - t_{j-1})/2$ . For the weight in (2) and for an affine invariant depth function,

$$W_{j} = \operatorname{vol}\{D_{\alpha}(F_{\mathbf{y}(t_{j}),N})\}(t_{j+1} - t_{j-1}) / \{\sum_{j=1}^{T} \operatorname{vol}\{D_{\alpha}(F_{\mathbf{y}(t_{j}),N})\}(t_{j+1} - t_{j-1})\}.$$

In the appendix we show that the finite sample MFD<sub>N</sub> can be written as a population MFD applied to a set of interpolating continuous K-dimensional processes  $\tilde{\mathbf{y}}$ , see (5), for which it holds that MFD<sub>N</sub>( $\mathbf{X}$ ) = MFD( $\mathbf{X}$ ;  $F_{\tilde{\mathbf{y}},N}$ ). The next theorem starts from the curves observed at a grid of time points and shows that the sample MFD is consistent for the population MFD under some conditions, when both N and T go to infinity.

**Theorem 3.** (Consistency) Let  $Y_1, \ldots, Y_N$  be a sample with the same distribution as  $\mathbf{\mathcal{Y}} \in \mathcal{C}(U)^K$  with  $E(\mathbf{\mathcal{Y}})$  finite. We only observe these curves at time points  $t_1 < \ldots < t_T$  from a design density  $f_T$  with  $G(t) = \int_{-\infty}^t f_T(u) du$  such that  $t_j = G^{-1}(\frac{j-1}{T-1})$  and that  $U = [G^{-1}(0), G^{-1}(1)]$  is compact. We assume that  $f_T$  is differentiable and that  $\inf_{t \in U} f_T(t) > 0$ . It holds that

$$\sup_{\boldsymbol{X} \in \mathcal{C}(U)^K} |MFD_N(\boldsymbol{X}) - MFD(\boldsymbol{X}; F_{\boldsymbol{y}})| \to 0, a.s. P,$$

as  $N \to \infty$  and  $T \to \infty$  when the statistical depth D is such that it satisfies the conditions of Definition 1, as well as (i)  $\sup_{\boldsymbol{x} \in \mathbb{R}^K} \left| D(\boldsymbol{x}; F_N) - D(\boldsymbol{x}; F) \right| \to 0$ , a.s. P, for  $F_N \to F$  as  $N \to \infty$  and (ii)  $\int_U \left| w(t; F_{\widetilde{\boldsymbol{y}}(t),N}) - w(t; F_{\boldsymbol{y}(t)}) \right| dt \to 0$  as  $N \to \infty$  a.s. P. For the weight function in (2), (ii) holds when  $P(\{\boldsymbol{x} \in \mathbb{R}^K : D(\boldsymbol{x}; F) = \alpha\}) = 0$ .

Halfspace depth satisfies condition (i) (Donoho and Gasko, 1992) and condition (ii) for the weight (2) at absolute continuous distributions (Mizera and Volauf, 2002).

Based on MFD<sub>N</sub> we can estimate the global pattern of the observed curves by means of the  $\Theta(t) \in \mathcal{C}(U)^K$  which attains maximal MFD<sub>N</sub>. For a general depth function D it might however be not straightforward to compute this median curve. In that case one can approximate  $\Theta(t)$  by the curve with maximal MFD<sub>N</sub> among all observed curves. Apart from estimating the global pattern of the curves, we are often interested in the variability of the curves. Our depth-based approach allows to visualize this dispersion by means of the central regions, introduced in López-Pintado and Romo (2009). The  $\beta$ -central region consists of the band delimited by the  $[n\beta]$  curves with highest depth. If we draw the 25%, 50% and 75% central regions, we obtain a representation of the data as in the enhanced functional boxplot of Sun and Genton (2011). See Section 3 and the supplementary material for examples. Based on these central regions, we define for each univariate set of curves their dispersion

curves  $s_{\beta}(t)$  as the width of the  $\beta$ -central region at each t. Note that the dispersion curves are defined on each of the univariate curves, but the underlying computation of the central regions is based on the MFD<sub>N</sub>. The  $t \mapsto s_{0.5}(t)$  dispersion curve can be considered as a kind of functional IQR, as explained in Sun and Genton (2011). A related concept, the scale curve, is defined in López-Pintado et al. (2010). It measures the area of the central region for  $\beta$  ranging from 0 to 1, and could be considered here as well. The  $\beta$ -trimmed mean and the  $\beta$ -trimmed variance (the mean and variance of all curves in the  $\beta$ -central region), see Fraiman and Muniz (2001), can be extended in a straightforward way too.

#### 2.3.2 Halfspace depth as a building block

As in the population case, we define the finite-sample multivariate functional halfspace depth (MFHD<sub>N</sub>) of a curve  $\boldsymbol{X} \in \mathcal{C}(U)^K$  as in Definition 3 with D the sample halfspace depth based on  $\{\boldsymbol{Y}_1(t), \dots, \boldsymbol{Y}_N(t)\}$  (Tukey, 1975),

$$\mathrm{HD}(\boldsymbol{X}(t); F_{\boldsymbol{\mathcal{Y}}(t),N}) = \frac{1}{N} \min_{\boldsymbol{u} \in \mathbb{R}^K, \|\boldsymbol{u}\| = 1} \# \{ \boldsymbol{Y}_n(t), n = 1, \dots, N : \boldsymbol{u}' \boldsymbol{Y}_n(t) \geqslant \boldsymbol{u}' \boldsymbol{X}(t) \}.$$

The finite-sample Tukey median is defined as the center of gravity of the deepest depth region. The median curve of the sample  $\{Y_1(t_j), \dots, Y_N(t_j); j = 1, \dots, T\}$  is defined as the Tukey median at each time point.

Exact computation of the MFHD<sub>N</sub> can be done with fast algorithms for the halfspace depth up to dimension K = 4 (Bremner et al., 2008). To compute the weight function (2), the algorithms developed in Hallin et al. (2010); Paindavaine and Šiman (2012) allow the computation of the depth contours up to dimension at least K = 5. In this paper we used the R-packages depth and aplpack which implement fast algorithms for bivariate and trivariate data (Rousseeuw and Ruts, 1996, 1998; Rousseeuw and Struyf, 1998; Rousseeuw et al., 1999). Approximate halfspace depth in higher dimensions can be computed by means of the random Tukey depth (Cuesta-Albertos and Nieto-Reyes, 2008), but it is no longer affine invariant.

To decide upon the value of  $\alpha$  in (2), one could consider some empirical quantile of the HD values at each time point, and take, e.g., their minimum or average. For example, if we set  $\alpha$  equal to the minimal median of the HD values, the resulting depth contours cover at least half of the data at each time point. Another possibility is to rely on the probability coverage of the depth contours, which can be computed exactly at some multivariate distributions. At bivariate normal data, it can be derived that  $\alpha = 1/8$  gives a coverage of 48% (Rousseeuw and Ruts, 1999). For univariate normal data, a 50% coverage is attained at  $\alpha = 1/4$ . We have used these as default values in our data examples and we have verified that the coverage was indeed around 50% at all time points.

# 3 Data examples

#### 3.1 Industrial data

We first illustrate our new depth function MFHD( $\alpha$ ) on an industrial data set that produces one part during each cycle (De Ketelaere et al., 2011). The behavior of the cycle as monitored by an accelerometer provides a fingerprint of the cycle and, related, of the quality of the produced part. If a deviating acceleration signal occurs, the process owner should be warned. Figure 2(a) shows the acceleration signal of N=224 parts measured during 120ms. Measurements are available every millisecond, hence the time signal ranges from  $t_1=1$  up to  $t_T=120$ . To augment this univariate data set, we could consider the derivatives of the curves as additional information, but in this example, we decided to use the integrated curves instead. As the velocity at time  $t_j$ ,  $V(t_j) = \int_{-\infty}^{t_j} A(t)dt$  with A(t) the acceleration at time t, we approximated the velocity by  $V(t_j) \approx V(t_{j-1}) + \{A(t_{j-1}) + A(t_j)\}/2$  starting with  $V(t_1) = 0$ . Note that the choice of the integration constant is not important here, due to the affine

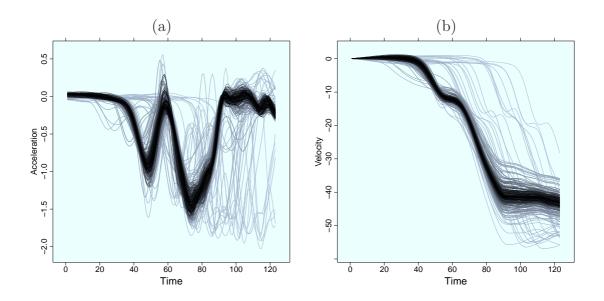


Figure 2: Industrial data: all signals colored according to their bivariate MFHD(1/8) depth.

invariance of MFHD( $\alpha$ ). The resulting velocity curves are depicted in Figure 2(b). Next, we performed a bivariate analysis on this data set, and computed the MFHD( $\alpha$ ) of all signals with  $\alpha=0.125$ . The resulting depth values can be visualized by means of the so-called rainbow plot (Hyndman and Shang, 2010). It shows the curves colored according to their MFHD value, going from dark grey for the deepest curve to light grey for the curve with minimal depth. Such a representation of the data is in particular useful to visualize potential outliers, as they are expected to have a lower MFHD depth and consequently should be colored light grey. In Figure 2 we see that the extreme outlying curves indeed are all colored light grey, which is a confirmation that our depth measure assigns them a low depth value.

Computing the MFHD on the bivariate data (A(t), V(t)) also yields the median curves, printed in black on Figure 1 for the acceleration and velocity curves. We see that these median curves are not attracted by the outlying values at the end of the cycle. Also the acceleration estimates in the valleys around time points 50 and 75 are

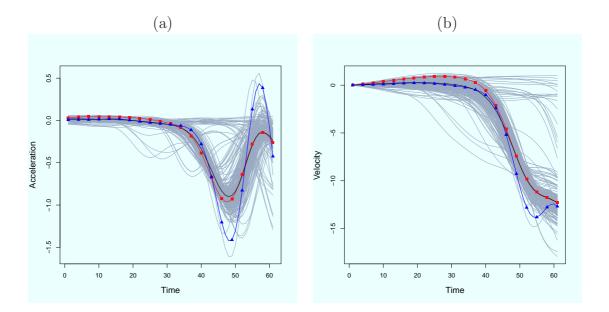


Figure 3: Industrial data: median curve (solid line), curve 7 (squares) and curve 82 (triangles).

lower than those of the mean curve, illustrating the robustness of the median curve towards the upward contamination values in these regions.

To illustrate the effect of the weight function, we restrict the data set to the first 61 ms. We focus on curve 7 (indicated with squares in Figure 3, and curve 82 (marked with triangles), and compute also their MFHD with a constant weight function. From Figure 3 it is obvious that curve 7 is not at all outlying and is very close to the MFHD median (solid line) in the second half of the time period where the amplitude is larger. Curve 82 is behaving well in the first phase, but becomes clearly outlying afterwards. This is well reflected in their MFHD(0.125) values, which achieve a large rank of 208 (out of 224) for curve 7 and a low rank of 34 for curve 82. When we ignore the differences in amplitude by using a constant weight, the depth of curve 7 has only rank 91, whereas curve 82 receives even a larger depth with rank 152. These depth values do not well reflect the position of the curves in the sample.

In the supplementary material we show the benefit of adding the velocity curves.

Some curves seem to be quite central when we only consider their acceleration, but become more outlying when adding their velocity. This not only affects the depth of the corresponding curves, but also the central regions and the dispersion curves.

#### 3.2 Weather data

In this section we present an example of bivariate functional data on which we illustrate the limited effect of outlying curves on the estimation of the MFHD median and the central regions. Our data set contains the temperature and dewpoint temperature (in degrees Celcius) measured between January 11 and 15, 2013 at 78 weather stations in the U.K. The raw data were downloaded from NOAA (www.noaa.gov). As different stations have different recording times, cubic spline interpolation was applied to obtain hourly estimates, yielding a total of 120 values, shown as the light grey curves in Figure 4(a) and (b). The dashed curves are the cross-sectional means which quite nicely reflect the general trend in the temperatures. On these data we applied MFHD with a constant weight function. Figures 4(c) and (d) show the resulting MFHD median and the boundaries of the 75% central regions by dashed curves.

Next we replaced eight curves with data from eight weather stations in Central Europe. They exhibit much lower temperatures as can be seen from the dark curves in Figure 4(a) and (b), and they affect the cross-sectional means heavily (depicted as solid lines). The solid lines in Figure 4(c) and (d) correspond to the MFHD median and the 75% central regions, computed on the contaminated data set. They are similar to the results based on the data from the U.K. only, which reflects the robustness of MFHD.

#### 4 Simulations

In this section we present three simulation settings each designed to illustrate a particular aspect of the behavior of MFHD. In all cases, we generate N = 50 univariate

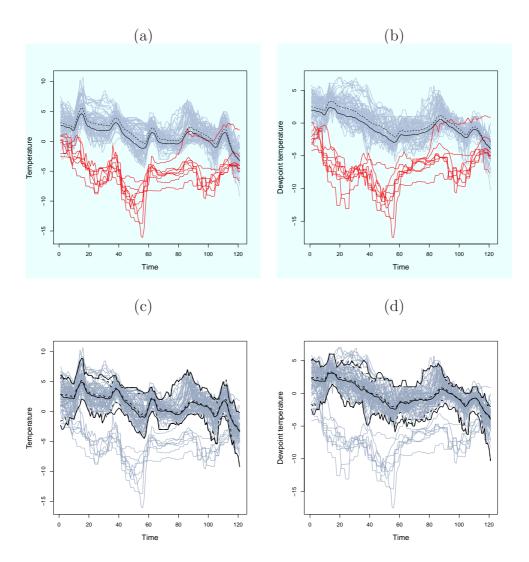


Figure 4: Weather data: (a)–(b) temperature and dewpoint temperature for weather stations in the U.K. (light grey) and Central Europe (dark) with cross-sectional means of the U.K. data only (dashed curves) and cross-sectional means of the full data set (solid curves); (c)–(d) MFHD median and central regions for the U.K. data only (dashed curves) and the full data set (solid curves).

curves  $\{Y_1(t), \ldots, Y_N(t)\}$  from a stochastic process  $\mathcal{Y}$ , denoted as the uncontaminated curves  $\{Y(t)\}_N$ . Then we replace five curves of  $\{Y(t)\}_N$  with curves sampled from a contaminating stochastic process  $\mathcal{Y}_{\varepsilon}$ , yielding a data set  $\{Y_1^{\varepsilon}(t), \ldots, Y_N^{\varepsilon}(t)\} = \{Y_{\varepsilon}(t)\}_N$  with 10% contamination. All curves are evaluated on a grid of T = 100 equispaced time points  $t_1, \ldots, t_T$  in  $[0, 2\pi]$ . Each experiment was replicated 100 times. In a first set of simulations (Section 4.2) we consider the bivariate MFHD applied to the curves and their derivatives. We compare its behavior with several univariate functional depths and with the bivariate random projection depth. Next, in Section 4.3 we illustrate the advantage of using the warping functions (or a function thereof) as additional curves. First we describe how we evaluate the performance and robustness of the functional depths.

#### 4.1 Evaluation criteria

ASE of the estimated central curve: the averaged squared scaled distance between the true and the estimated central curve,

$$\frac{1}{T} \sum_{j=1}^{T} \left( \frac{\widehat{m}_{Y_{\varepsilon}}(t_j) - m_{\mathcal{Y}}(t_j)}{s_{\mathcal{Y}}(t_j)} \right)^2,$$

where  $m_{\mathcal{Y}}$  is the central curve of  $\mathcal{Y}$ ,  $\widehat{m}_{Y_{\varepsilon}}$  is the estimated central curve, and  $s_{\mathcal{Y}}(t)$  is the interquartile range of  $\mathcal{Y}(t)$ .

ASE of the estimated dispersion curve: the average squared difference between the logarithm of the (0.5)-dispersion curves computed on the contaminated and the uncontaminated data,

$$\frac{1}{T} \sum_{j=1}^{T} \left( \log \left( \frac{s_{0.5}^{\varepsilon}(t_j)}{s_{0.5}(t_j)} \right) \right)^2,$$

where  $s_{0.5}(t)$  is the width of the (0.5)-central region of  $\{Y(t)\}_N$  as defined in Section 2.3. Analogously,  $s_{0.5}^{\varepsilon}(t)$  is the dispersion curve computed from  $\{Y_{\varepsilon}(t)\}_N$ .

Normalized maximum depth of outliers. To have an easily comparable criterion, we normalize by dividing the maximum depth with the depth of the deepest curve.

Formally, let  $\mathrm{FD}_N(Y_n^{\varepsilon}, F_{\mathcal{Y}_{\varepsilon},N})$  denote the (finite-sample) functional depth of the curves  $Y_n^{\varepsilon}(t)$  from  $\{Y_{\varepsilon}(t)\}_N$ , and denote by  $I_c$  the index set of the contaminated curves from  $\{Y_{\varepsilon}(t)\}_N$ . Then we consider  $\max_{n\in I_c}\mathrm{FD}_N(Y_n^{\varepsilon}, F_{\mathcal{Y}_{\varepsilon},N})/\max_{n=1,\dots,N}\mathrm{FD}(Y_n^{\varepsilon}, F_{\mathcal{Y}_{\varepsilon},N})$ .

#### 4.2 Simulations with curves and their derivatives

We generate three types of univariate curves, contaminated with 10% outlying curves, and we evaluate MFHD on the bivariate samples  $\{(Y_{\varepsilon}(t), Y'_{\varepsilon}(t))\}_N$ . We consider both  $\alpha = 1/4$  and  $\alpha = 1/8$ , resulting in MFHD(1/4) and MFHD(1/8). In both cases the estimated central curve  $\hat{m}_{Y_{\varepsilon}}(t)$  is the MFHD median, as in Definition 2.

We compare the behavior of MFHD on the bivariate samples, first, with three approaches applied on the univariate curves  $\{Y_{\varepsilon}(t)\}_{N}$ . (1) The cross-sectional average (CSA):  $\widehat{m}_{Y_{\varepsilon}}(t) = \frac{1}{50} \sum_{n=1}^{50} Y_{n}^{\varepsilon}(t)$ . The corresponding depth is the univariate Mahalanobis depth, with  $\widehat{\sigma}_{Y_{\varepsilon}}(t)$  the cross-sectional standard deviation,

$$MD(Y_n^{\varepsilon}(t)) = \left\{ 1 + \left( \frac{Y_n^{\varepsilon}(t) - \widehat{m}_{Y_{\varepsilon}}(t)}{\widehat{\sigma}_{Y_{\varepsilon}}(t)} \right)^2 \right\}^{-1}.$$

(2) The modified band depth (MBD) of López-Pintado and Romo (2009). This corresponds with MFD( $Y_i, \mathcal{Y}_{\varepsilon}$ ) as in (4) with the simplicial depth (Liu, 1990) as depth function D and with constant weight function w(t) = 1/T. The curve with largest MBD is considered as  $\widehat{m}_{Y_{\varepsilon}}(t)$ . We use the implementation provided in the R package depthtools. (3) The MFHD( $\alpha = 1/4$ ) applied to the univariate curves  $\{Y_{\varepsilon}(t)\}_{N}$ , which we denote by UFHD(1/4). Note that the deepest curve in this case corresponds to the cross-sectional median.

Next, we compare with the bivariate random projection depth (RPD) of Cuevas et al. (2007), using the default settings from the implementation in the R package fda.usc (Febrero-Bande and Oviedo de la Fuente, 2012). Here, the curves and their derivatives are projected on a random direction, yielding a bivariate sample on which the (bivariate) modal depth (Cuevas et al., 2006) can be computed for all observations.

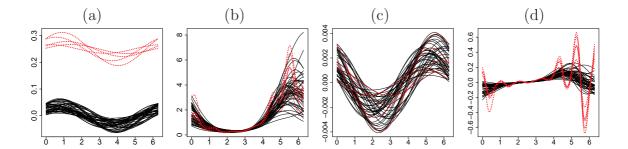


Figure 5: Simulation settings. Main curves (solid) and outliers (dashed) for the curves (a),(b) and their derivatives (c),(d) for (a),(c) the shifted outliers; (b),(d) the log-normal processes.

The RPD of a curve corresponds with the average modal depth over 50 random projections. Note that this approach does not satisfy the affine invariance property as stated in Theorem 1.

The functional derivatives are computed using B-splines using the default settings and the algorithms from the R-package fda.usc.

#### 4.2.1 Simulation setting I: Shifted outliers

This simulation setting illustrates the behavior of MFHD in cases where the true curves are homoscedastic and all derivative curves follow the same process. We generated curves of the form

$$Y_n^{\varepsilon}(t) = (1 - c_n)\{a_{1n}\sin(t) + a_{2n}\cos(t)\} + c_n\{a_{1n}\sin(t) + a_{2n}\cos(t) + \frac{1}{4}\},\$$

where t is a grid of 100 equispaced values on  $[0, 2\pi]$ ,  $c_n$  is 1 for 10% of the curves and 0 otherwise. The random coefficients  $a_{1n}$  and  $a_{2n}$  follow independent uniform distributions on [0, 0.05]. Figure 5(a) depicts the 'regular' (solid) and outlying (dashed) curves and Figure 5(d) the corresponding derivatives.

The first panel in Figure 6 depicts, for each of the functional depth methods, the ASE of the central curves. CSA is highly influenced by the outlying curves, and RPD

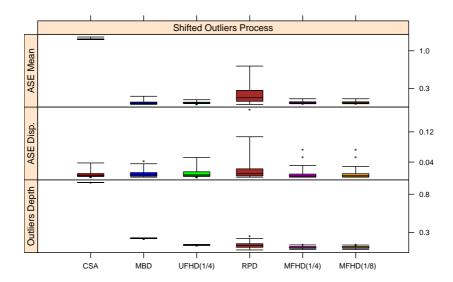


Figure 6: Setting I: shifted outliers. ASE of the estimated central curve (top), of the 0.5-dispersion curve (middle) and outlier depth (bottom).

to a lesser extend. The middle panel in Figure 6 depicts the ASE of the dispersion curve. The effects of the outliers on the CSA estimate of dispersion  $s_{0.5}(Y_n^{\varepsilon}(t))$  is more muted because the outlying curves are located too far to be included in the set of 25 curves with largest Mahalanobis depth. RPD contains some large values too. All other methods perform well on both criteria. The third panel in Figure 6 depicts the (normalized) maximum depth of outliers. Here again, CSA assigns a high depth to the outliers. Both univariate functional depths (MBD and UFHD) assign higher depths to the outliers than the bivariate depth functions. The value of  $\alpha$  for MFHD( $\alpha$ ) has a negligible effect on all three performance criteria.

#### 4.2.2 Simulation setting II: Log-normal processes

Highly heteroscedastic curves are obtained by generating from a log-normal process  $Y_n(t) \sim \log N(\mu(t), \Sigma(t))$ . Denote  $\boldsymbol{x} = \{x_i\}_{i=1}^{20}$  20 equidistant points on  $[0, 2\pi]$ . The covariance kernel of the  $x_i$ 's is given by  $K_{xx}(i,j) = \exp\left(-\frac{(x_j-x_i)^2}{2\delta^2}\right)$ , with  $\delta = 0.25$ . For the time points  $\boldsymbol{t} = \{t_j\}_{j=1}^{100}$  equidistant on  $[0, 2\pi]$ , we define  $K_{tx}$  and

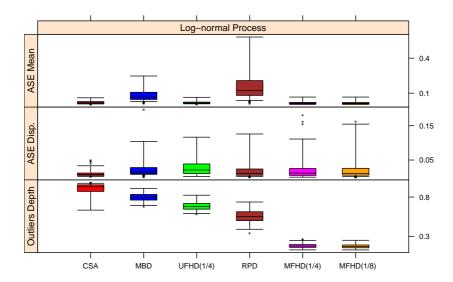


Figure 7: Setting II: log-normal processes. ASE of the estimated central curve (top), of the 0.5-dispersion curve (middle) and outlier depth (bottom).

 $K_{tt}$  analogously. Then, the weight matrix for the mean  $\mu$  is  $K^m = K_{tx}(K_{xx} + D)^{-1}$  where D is a diagonal matrix that directs the heteroscedasticity of the final process,  $D = \text{Diag}_{i=1,\dots,20}\{\min((\pi - x_i)^2, 1)\}$ , so that the variance of the process is minimized at  $t = \pi$ . For the regular curves we take  $\mu(t) = K^m(a_1 \sin(x) + a_2 \cos(x))$ , where  $a_1 \sim \mathcal{U}(-2,2)$  and  $a_2 \sim \mathcal{U}(-1,1)$  are randomly generated. For the outlying curves we took  $\mu^*(t) = K^m(\sin(6x) + \mu(x))$ . The covariance matrix is given by  $\Sigma = K_{tt} - K_{tx}(K_{xx} + D)^{-1}K'_{tx}$ . For a generated sample of curves and the corresponding derivatives, see Figure 5(c),(f).

This configuration was designed to penalize those estimators that do not use the information from the derivatives of the curves to assign depths. This is particularly visible in the third panel of Figure 7, where the CSA, MBD, UFHD and RPD are unable to detect the outlying curves. The outliers do not affect the CSA in terms of ASE of the central and the dispersion curves since the range of the response values is the same for all curves. Although RPD uses the derivatives, it does not perform

well; RPD is not estimating the central curve well, and it does not assign low depths to the outlying curves. MFHD retains its good behavior.

#### 4.3 Simulation with warped curves

Warping can make outlying curves more difficult to detect by pulling them towards the uncontaminated ones. See Figure 8 for an example where outlying curves are initially visible but are then hidden by the warping process. Here, using a bivariate approach can help with the ranking of the curves. For MFHD we compare two bivariate approaches. First, we create a bivariate sample of curves by using the warped curves together with the individual warping functions. Second, we use as a bivariate sample of curves the warped curves together with the derivatives of the warping functions. Adding the curves related to warping alleviates the information loss induced by the warping procedure.

For the warping functions, our simulation design follows that used in the first simulation setting of Arrabis-Gil and Romo (2012). The warping functions for the good curves are generated as explained on their page 405, formula (3.7). The inverse of

$$h_n(t) = \frac{\arctan(\beta_n(2t-1))}{2\arctan(\beta_n)} + 1/2, \ t \in [0,1]$$

with  $\beta_n$  equally spaced between 10 and 14 is used as warping function for the outliers. We use the same amplitude functions for all curves such that different warping functions correspond to original curves with different shapes and phases. To make the results comparable with those of simulation setting I, we use  $Y_n(t) = a_{1i}\sin(t/(2\pi)) + a_{2i}\cos(t/(2\pi))$ . A sample of curves and warped curves is depicted in Figure 8, together with the warping functions and their derivatives.

For comparison we use two versions for UFHD: only the unwarped curves, and only the warped curves. Figure 9 contains a summary of the performance criteria.

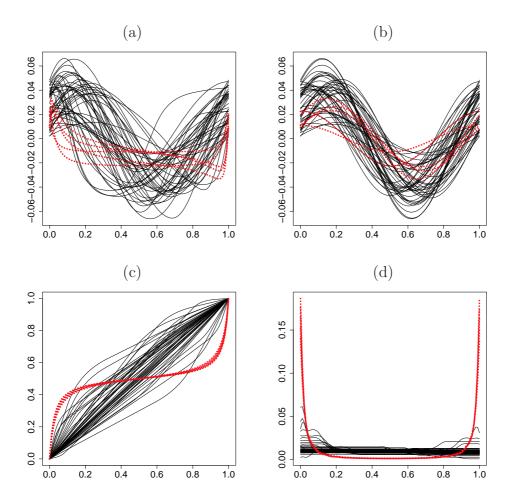


Figure 8: Simulation setting III. (a) Original curves, (b) warped curves, (c) warping functions, (d) derivatives of the warping functions; outlying curves as dashed lines.

As expected, once warped, the outlying curves have no influence on the estimation of the central (or dispersion curves) and this is visible in the first two panels of Figure 9 where UFHD has low MSE on both measures. At the same time, warping makes the curves with different shapes similar to the other curves, causing a poor behavior of UFHD on the warped curves in the third panel. Adding the warping functions, or their derivatives in a bivariate analysis completely addresses the information loss introduced by the warping procedure.

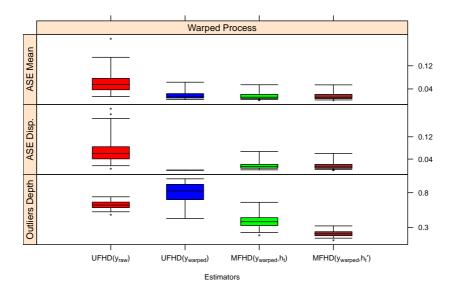


Figure 9: Setting III. ASE of the estimated central curve (top) and the 0.5-dispersion curve (middle) and outlier depth (bottom). Using the original curves  $(y_{\text{raw}})$ , the warped curves  $(y_{\text{warped}})$  and their warping functions  $(h_t)$  with derivatives  $h'_t$ .

## 5 Discussion

We have presented a new depth function for multivariate functional data (MFD), defined as a weighted average of the cross-sectional multivariate depths. It assigns a ranking to curves from the center outwards, whilst accounting for differences in amplitude. Shape and phase variation can be accommodated by including derivatives and/or warping functions. Interesting theoretical properties and computational advantages are achieved when using the multivariate halfspace depth, which leads to the MFHD depth function. The multivariate functional median curve can then be computed explicitly and estimates the central behavior of the curves. MFHD also allows to visualise and quantify the variability amongst the curves. Simulations have shown the benefit of adding derivatives or warping information to univariate curves, and they have illustrated the better performance of MFHD compared with the bivariate random projection depth.

Depth functions are regularly used for the classification and clustering of multivariate data, see e.g. Ghosh and Chaudhuri (2005), Dutta and Ghosh (2011), Hubert and Van der Veeken (2010), Jörnsten (2004). This has been extended to the classification of functional data, as in Cuevas et al. (2007), López-Pintado and Romo (2006) and Hlubinka and Nagy (2012). It will be interesting to study the use of MFHD for the classification of multivariate curves, as well as for the classification of univariate curves augmented with their derivatives or warping functions. Some preliminary results indicate that this will indeed be beneficial (Slaets, 2011). Combining MFDH with the DD-plot of Li et al. (2012) is another interesting topic of further research. We will also investigate the possible use of MFHD for online quality control.

As illustrated in the data examples and in the simulations, MFHD assigns lower depth to curves which deviate strongly from the majority of the curves. This robustness towards outliers is inherited from the halfspace depth which is applied at every time point. It is however well known that other depth functions, such as projection depth (Zuo, 2003) and spatial depth (Serfling, 2002), attain a higher breakdown value and thus could lead to a more robust MFD. Alternatively one could replace the integral in (1) (or equivalently the average in (4)) by an infimum as proposed in Mosler and Polyakova (2012). More theoretical and numerical studies are needed to compare these different depth functions.

# A Appendix – Proofs of Section 2

## Proof of Theorem 1

*Proof.* (i) For a depth function D that is affine invariant and for weight function (2) use that  $\operatorname{vol}\{D_{\alpha}(\boldsymbol{\mathcal{Y}}(t))\} = |\det(\boldsymbol{A})| \cdot \operatorname{vol}(D_{\alpha}\{\boldsymbol{A}\boldsymbol{\mathcal{Y}}(t) + \boldsymbol{X}(t))\}$ , to obtain the affine invariance for MFD. (ii) – (iv) are immediate from the assumptions on D.

#### Proof of Theorem 2

*Proof.* (i) and (ii) These parts of the theorem follow by application of Theorems 2 and 3 of Ausubel and Deneckere (1993). (iii) Trivial.

(iv) We prove by contradiction that a deepest curve implies deepest points at every  $t \in U$ . Suppose that there exists a  $t_1 \in U$  with  $D(\vartheta(t_1); F_{\boldsymbol{\mathcal{Y}}(t_1)}) < D(\Theta_{t_1}; F_{\boldsymbol{\mathcal{Y}}(t_1)})$  for  $\Theta_{t_1} \in \Theta(t_1)$ . Since by (i) or (ii)  $\Theta$  is compact-valued, there exists an open neighborhood B of  $\vartheta(t_1)$ , and an open neighborhood C of  $\Theta(t_1)$  such that  $B \cap C = \emptyset$ . Since  $\vartheta$  is continuous, there exists a  $\delta_1 > 0$  such that for  $|t - t_1| < \delta_1$ :  $\vartheta(t) \in B$ . By the upper-hemicontinuity of  $\Theta$ , there exists a  $\delta_2 > 0$  such that for  $|t - t_1| < \delta_2$ :  $\Theta(t) \subset C$ . Take  $\delta = \min\{\delta_1, \delta_2\}$ . Then, since  $B \cap C = \emptyset$ , for  $|t - t_1| < \delta$ ,  $D(\vartheta(t); F_{\boldsymbol{\mathcal{Y}}(t)}) < D(\Theta_t; F_{\boldsymbol{\mathcal{Y}}(t)})$  for  $\Theta_t \in \Theta(t)$ , and thus

$$MFD(\boldsymbol{\vartheta}; F_{\boldsymbol{\mathcal{Y}}}) = \int_{U} D(\boldsymbol{\vartheta}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) w(t) dt$$

$$< \int_{|t-t_{1}| \geq \delta} D(\boldsymbol{\Theta}_{t}; F_{\boldsymbol{\mathcal{Y}}(t)}) w(t) dt + \int_{|t-t_{1}| < \delta} D(\boldsymbol{\Theta}_{t}; F_{\boldsymbol{\mathcal{Y}}(t)}) w(t) dt$$

which is in contradiction with the fact that  $\vartheta$  is a deepest curve.

#### Finite sample MFD. Calculation of (4)

In order to apply Definition 1 to the curve observations at a grid of time points, we use linear interpolation on each interval  $[t_j, (t_j + t_{j+1})/2]$  to connect the values  $(t_j, Y_{nk}(t_j))$  with the average of the function values at time  $t_j$  in the middle of the time interval  $((t_j + t_{j+1})/2, \bar{Y}_k(t_j) = N^{-1} \sum_{n=1}^N Y_{nk}(t_j))$ , for  $j = 1, \ldots, T-1$  and for each  $k = 1, \ldots, K$ . Similarly, for  $j = 1, \ldots, T-1$ , on the interval  $[(t_j + t_{j+1})/2, t_{j+1}]$ , linear interpolation is used to connect the values  $((t_j + t_{j+1})/2, \bar{Y}_k(t_j))$  and  $(t_{j+1}, Y_{nk}(t_{j+1}))$ . This yields a sample of continuous K-dimensional processes  $\tilde{\boldsymbol{\mathcal{Y}}}_n$ ,  $n = 1, \ldots, N$  on the

interval  $[t_1, t_T]$  of which the kth component (k = 1, ..., K) is defined by

$$\widetilde{\mathbf{y}}_{n,k}(t) = \begin{cases}
Y_{nk}(t_j) \frac{t_j + t_{j+1} - 2t}{t_{j+1} - t_j} + \bar{Y}_k(t_j) \frac{2(t - t_j)}{t_{j+1} - t_j} & \text{for } t \in [t_j, (t_j + t_{j+1})/2] \\
-Y_{nk}(t_{j+1}) \frac{t_j + t_{j+1} - 2t}{t_{j+1} - t_j} - \bar{Y}_k(t_j) \frac{2(t - t_{j+1})}{t_{j+1} - t_j} & \text{for } t \in [(t_j + t_{j+1})/2, t_{j+1}].
\end{cases} (5)$$

The empirical cumulative distribution function of this sample is denoted by  $F_{\widetilde{\boldsymbol{y}},N}$ . Note that the definition of the K-variate processes  $\widetilde{\boldsymbol{\mathcal{Y}}}_n$  depends on both N and T. Using the definition of MFD on population level, see (1), with the processes  $\widetilde{\boldsymbol{\mathcal{Y}}}_n$ , and the affine invariance of D, with  $t_0 = t_1$  and  $t_T = t_{T+1}$  gives Definition 3. Indeed,

$$MFD(\mathbf{X}; F_{\widetilde{\mathbf{y}},N}) = \sum_{j=1}^{T-1} \left\{ D(\mathbf{X}(t_j); F_{\mathbf{y}(t_j),N}) \int_{t_j}^{(t_j + t_{j+1})/2} w(t) dt + D(\mathbf{X}(t_{j+1}); F_{\mathbf{y}(t_{j+1}),N}) \int_{(t_j + t_{j+1})/2}^{t_{j+1}} w(t) dt \right\}$$

$$= D(\mathbf{X}(t_1); F_{\mathbf{y}(t_1),N}) \int_{t_1}^{(t_1 + t_2)/2} w(t) dt$$

$$+ \sum_{j=2}^{T-1} D(\mathbf{X}(t_j); F_{\mathbf{y}(t_j),N}) \int_{(t_{j-1} + t_j)/2}^{(t_j + t_{j+1})/2} w(t) dt$$

$$+ D(\mathbf{X}(t_T); F_{\mathbf{y}(t_T),N}) \int_{(t_{T-1} + t_T)/2}^{t_T} w(t) dt.$$

#### Proof of Theorem 3

Proof. On the space of curves in  $\mathcal{C}(U)^K$  we define the uniform distance  $\rho(X,Y) = \sup_{t \in U} \|X(t) - Y(t)\|$ , with  $\|\cdot\|$  the Euclidean norm in  $\mathbb{R}^K$ . We first show that the functions  $\{\widetilde{\boldsymbol{\mathcal{Y}}}_n : U \to \mathbb{R}^K : t \mapsto \widetilde{\mathcal{Y}}_{n,1}(t), \dots, \widetilde{\mathcal{Y}}_{n,K}(t), n = 1, \dots, N\}$  for  $N \to \infty$  and  $T \to \infty$  converge weakly to  $\boldsymbol{\mathcal{Y}}$ . Since  $E(\boldsymbol{\mathcal{Y}})$  is finite, the law of large numbers implies that for each  $t \in U$  and for  $k = 1, \dots, K$ ,  $\bar{Y}_k(t) = N^{-1} \sum_{n=1}^N Y_{nk}(t) \to_{N \to \infty} E[\mathcal{Y}_k(t)]$ , a.s.

By the design assumption,  $|t_{j+1} - t_j| = |(G^{-1})'(\xi_j)|/(T-1) = c_j/(T-1)$ , for a constant  $c_j$  and  $\xi_j$  in between  $t_j$  and  $t_{j+1}$ . For each  $t \in U$  there is precisely one interval  $[t_j, t_{j+1})$  that contains t and since the interpolating process agrees with the observed

curve on the time points  $t_1, \ldots, t_T$ , it follows that for each value  $n = 1, \ldots, N$ ,

$$0 \leqslant \rho(\widetilde{\boldsymbol{\mathcal{Y}}}_n, \boldsymbol{Y}_n) \leqslant 2 \sup_{|s-t| \leqslant c/(T-1)} \|\boldsymbol{Y}_n(t) - \boldsymbol{Y}_n(s)\| = 2w_{\boldsymbol{Y}_n}(c/(T-1)),$$

with  $w_{\boldsymbol{Y}}$  the modulus of continuity of  $\boldsymbol{Y}$  and with  $c=1/\inf_{t\in U}f_T(t)$ . Since U is compact and each function  $\boldsymbol{Y}_n$  is continuous, this function is also uniformly continuous and thus  $w_{\boldsymbol{Y}_n}(c/(T-1)) \to 0$  as  $T \to \infty$ . Since the sample of curves is i.i.d. and by Theorems 3.2 and 7.5 of Billingsley (1999), there is weak convergence of the interpolating processes  $\widetilde{\boldsymbol{\mathcal{Y}}}_N$  to  $\boldsymbol{\mathcal{Y}}$  as  $N \to \infty$  and  $T \to \infty$ . It holds that

$$\sup_{\boldsymbol{X} \in \mathcal{C}(U)^K} \left| \mathrm{MFD}(\boldsymbol{X}; F_{\widetilde{\boldsymbol{y}}, N}) - \mathrm{MFD}(\boldsymbol{X}; F_{\boldsymbol{y}}) \right| \leqslant$$
(6)

$$\sup_{\boldsymbol{X} \in \mathcal{C}(U)^K} \int_{U} \left| D(\boldsymbol{X}(t); F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N}) - D(\boldsymbol{X}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) \right| dt + \int_{U} \left| w(t; F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N}) - w(t; F_{\boldsymbol{\mathcal{Y}}(t)}) \right| dt.$$

The convergence to zero of the first integral is obtained by rewriting the integration over U as a sum of integrals over the domains in (5). For  $T \in [t_j, (t_j + t_{j+1}))/2$ , e.g., use that  $\left| D(\boldsymbol{X}(t); F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N}) - D(\boldsymbol{X}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) \right| \leq \left| D(\boldsymbol{X}(t_j); F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N}) - D(\boldsymbol{X}(t_j); F_{\boldsymbol{\mathcal{Y}}(t)}) \right| + \left| D(\boldsymbol{X}(t_j); F_{\boldsymbol{\mathcal{Y}}(t)}) - D(\boldsymbol{X}(t); F_{\boldsymbol{\mathcal{Y}}(t)}) \right|$ , where we used the constancy of the finite sample depth on each such interval by definition of  $\widetilde{\boldsymbol{\mathcal{Y}}}_N$ . The weak convergence of  $\widetilde{\boldsymbol{\mathcal{Y}}}_N$  to  $\boldsymbol{\mathcal{Y}}$  as  $N \to \infty$ , together with the boundedness of the depth, the design and the fact that the set of interval endpoints has measure zero, ends the proof.

We now prove condition (ii) for the weight in (2). Under the stated assumptions, Theorem 4.1 of Zuo and Serfling (2000b) yields the a.s. convergence of the  $\alpha$ -trimmed regions  $D_{\alpha}(F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N})$  to  $D_{\alpha}(F_{\boldsymbol{\mathcal{Y}}(t)})$ , together with a nesting property such that for  $0 < \epsilon < \alpha$ ,  $D_{\alpha}(F_{\widetilde{\boldsymbol{\mathcal{Y}}}(t),N}) \subset D_{\alpha-\epsilon}(F_{\boldsymbol{\mathcal{Y}}(t)})$  for all  $t \in U$ . By the dominated convergence, the right-hand side of (6) converges to 0 a.s. P as  $N, T \to \infty$ .

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# Multivariate Functional Halfspace Depth Supplementary Materials

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## 1 Univariate versus bivariate analysis of the industrial data

We illustrate on the industrial data set the benefit of adding the integrated curves (here, the velocity curves) to the analysis. Figures 1(c) and (e) show the 25%, 50% and 75% central regions of the acceleration and velocity curves, based on the bivariate MFHD(1/8) depth (with the MFHD median superimposed in white). Their cross-sectional width yields the dispersion curves in Figures 1(d) and (f). When we only consider the acceleration data and set  $\alpha=1/4$ , the multivariate halfspace depth reduces to the weighted average of the univariate halfspace depth, which we denote by UFHD(1/4). We then obtain the UFHD median and the central regions displayed in Figure 1(a). The UFHD median is identical to the cross-sectional median and does not differ much from the MFHD median. We notice that the 50% and 75% central regions of the acceleration curves are quite different between 40ms and 60ms. This behavior is also reflected in the dispersion curves in Figure 1(a). Note that all the dispersion curves clearly expose the heteroscedasticity of both the acceleration and velocity signals, and they give an indication of the amount of outlying signals.

To understand the difference between the univariate and the bivariate analysis, we first compare the univariate UFHD(1/4) and bivariate MFHD(1/8) values for all curves, shown in Figure 2. We observe a global monotone trend showing that curves with a low UFHD depth also have a low MFHD depth, but the relation is certainly not strictly monotone. Changing  $\alpha$  did not make a substantial difference in UFHD or MFHD.

Let us focus on one specific deviating curve, with label 112, indicated by the dotted

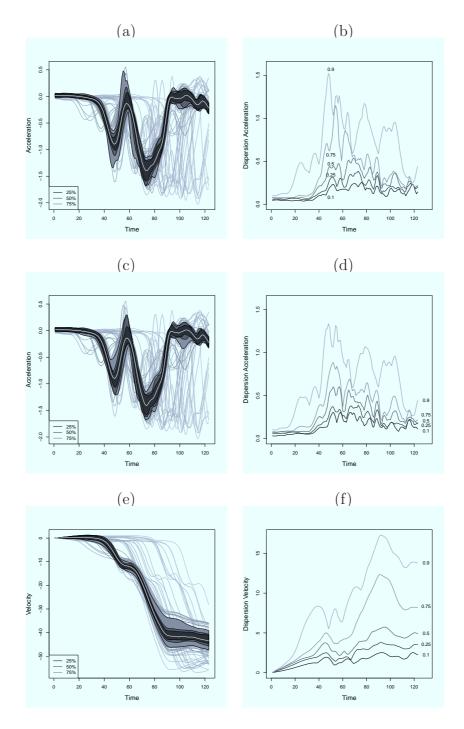


Figure 1: Central regions and dispersion curves for: (a)–(b) the acceleration curves based on UFHD(1/4), (c)–(d) the acceleration curves based on MFHD(1/8), (e)–(f) the velocity curves based on MFHD(1/8).

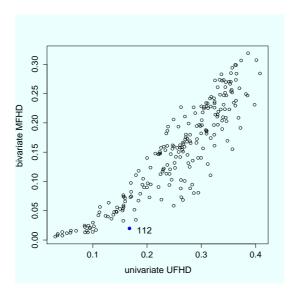


Figure 2: Acceleration data: bivariate MFHD(1/8) versus univariate UFHD(1/4).

line in Figure 3, for comparison together with the deepest curve. From Figure 3(a) we notice that it attains larger acceleration values at the peaks around 47ms and 57ms, and one additional oscillation between 60ms and 80ms. Consequently its univariate depth, only based on this information, is somewhat lower but it is not extremely small. To be more precise, the univariate UFHD of curve 112 has rank 45 (out of 224). When we include the information given by the velocity curves, we see from Figure 3(b) that the velocity of curve 112 is outlying on almost the whole time domain. This yields a bivariate MFHD with rank 15. As a result, the 75% central region based on the bivariate depth does not include the curves with large peaks around 47ms and 57ms, whereas the univariate-based central region does include them.

# 2 Discontinuity of the MFHD median

Theorem 2 states several conditions that are required for the MFHD median to be continuous. The following counter example shows that only continuity of the process  $\mathcal{Y}$  is not sufficient.

Consider a bivariate stochastic process on U = [0, 1] which is an equal weighted

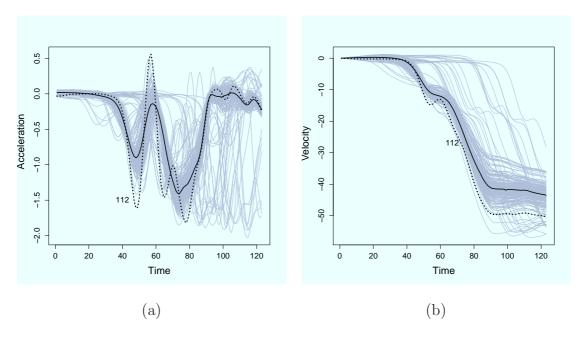


Figure 3: (a) Acceleration and (b) velocity curves with one outlying curve (dotted line) and the median curve (solid line).

mixture of three possible paths X(t), Y(t) and Z(t). The constant functions X(t) and Y(t) are X(t) = (0,0) and Y(t) = (0,1), whereas Z(t) = (t-0.5,0). Note that the Tukey median is unique at each time point. For  $t \neq 0.5$  the Tukey median equals (1/3(t-0.5), 1/3) being the center of gravity of the triangle with coordinates (0,0), (0,1) and (t-0.5,0). Its depth is 1/3. For  $t \to 0.5$  this median converges to (0,1/3). However at t=0.5 the Tukey median is (0,0) and has depth 2/3. The bivariate curve with maximal HD depth, as well as the maximal depth function are thus not continuous.

Considering the set of assumptions (a) in Theorem 2, the correspondence  $\Pi$  is not lower-hemicontinuous at t=0.5 in this case, only assuming continuity of the processes. Indeed,

$$\Pi: [0,1] \to \mathbb{R}: t \mapsto \begin{cases} (-\infty, 1/3] & \text{for } t \neq 0.5\\ (-\infty, 2/3] & \text{for } t = 0.5. \end{cases}$$

Take for example the open interval (0.5, 5/6), which has a non-empty intersection

with  $\Pi(0.5)$ . For any open neighborhood of t=0.5, for all  $x\in[0,1]$  in this open neighborhood with  $x\neq 0.5$ , it holds that  $\Pi(x)\cap V=\emptyset$ . Analogously, for the set of assumptions (b), it can be shown that  $\widetilde{G}$  is not continuous in t=0.5.