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This is an **author produced version** of a paper published in:

Advances in Data Analysis and Classification (2015): 1-20

DOI: <http://dx.doi.org/10.1007/s11634-015-0217-7>

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On visual distances for spectrum-type functional data

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Abstract

A functional distance \mathbb{H} , based on the Hausdorff metric between the function hypographs, is proposed for the space \mathcal{E} of non-negative real upper semicontinuous functions on a compact interval. The main goal of the paper is to show that the space $(\mathcal{E}, \mathbb{H})$ is particularly suitable in some statistical problems with functional data which involve functions with very wiggly graphs and narrow, sharp peaks. A typical example is given by spectrograms, either obtained by magnetic resonance or by mass spectrometry. On the theoretical side, we show that $(\mathcal{E}, \mathbb{H})$ is a complete, separable locally compact space and that the \mathbb{H} -convergence of a sequence of functions implies the convergence of the respective maximum values of these functions. The probabilistic and statistical implications of these results are discussed in particular, regarding the consistency of k -NN classifiers for supervised classification problems with functional data in \mathbb{H} . On the practical side, we provide the results of a small simulation study and check also the performance of our method in two real data problems of supervised classification involving mass spectra.

Key words: Supervised classification, functional data analysis, Hausdorff metric.

1 Introduction: the choice of a suitable functional distance

The statistical analysis of problems where the sample data are functions is often called Functional Data Analysis (FDA). This is a relatively new statistical field which involves several specific challenges, most of them are associated with the infinite-dimensional nature of the data.

We are concerned here with one of these specific challenges, namely, the choice of a suitable distance criterion between the data. In what follows,

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unless otherwise stated, we will consider problems where the sample data are real functions $x(t)$, $t \in [0, 1]$.

Not surprisingly, a considerable part of the current FDA theory has been developed assuming that the data functions belong to the space $L^2[0, 1]$, that is, the distance between two data x_1 and x_2 is given by $d_2(x_1, x_2) = (\int_0^1 (x_1(t) - x_2(t))^2 dt)^{1/2}$. This distance presents obvious advantages, derived from the fact that $L^2[0, 1]$ is a Hilbert space. Thus, some extremely important tools, as the existence of orthogonal bases (and the corresponding expansions for the data in orthogonal series) are available in $L^2[0, 1]$. As a useful by-product, some crucial methodologies, such as Principal Components Analysis or Linear Regression (and even Partial Least Squares), can be partially adapted to the functional setting.

Another widely used metric is associated with the supremum norm $\|x\|_\infty = \sup_t |x(t)|$, which is well-defined in the space $\mathcal{C}[0, 1]$ of real continuous functions $x : [0, 1] \rightarrow \mathbb{R}$; thus the metric is $d_\infty(x_1, x_2) = \sup_t |x_1(t) - x_2(t)|$ for $x_1, x_2 \in \mathcal{C}[0, 1]$. Although the Hilbert structure is lost here, the advantages of the supremum metric are also well-known: first, d_∞ is easy to interpret in terms of vertical distance between the functions. Second, the structure of the space of probability measures on $(\mathcal{C}[0, 1], \|\cdot\|_\infty)$ is also well understood, and carefully analyzed, for example, in the classical book by Billingsley (1968).

For general accounts on the FDA theory we refer to the books by Bosq (2000), Bosq and Blanke (2007), Ramsay and Silverman (2002, 2005), Ferraty and Vieu (2006), Horváth and Kokoszka (2012) and the recent survey paper by Cuevas (2014).

1.1 Our proposal: its practical motivation

In what follows we analyze, from both the theoretical and practical point of view, a metric between functions especially aimed at capturing the “visual distance” between the graphs. This metric will be particularly suitable in FDA problems where the data are functions with wiggly graphs showing very sharp peaks. In those situations the classical metrics (d_2 or d_∞) could be unsuccessful in capturing a “practically meaningful” notion of distance between the graphs. For example, a small lateral shift in a very sharp peak (perhaps due to a registration error) could lead to an enormous d_∞ -distance. Likewise, if two graphs differ in just one such narrow peak, the d_2 -distance between them might be very small, which could be unsuitable in many cases.

The spectrograms, either obtained from magnetic resonance ($^1\text{H-NMR}$ or $^{13}\text{C-NMR}$) or by mass spectrometry, provide a good example of such situations. Just as an example to motivate our point, let us consider the $^{13}\text{C-NMR}$ spectrum of a compound, namely the o-xylene (C_8H_{10}); see Figure 1, left.

It shows the typical spiky pattern, with sharp and narrow peaks, strongly localized (we will consider below other examples of much more complex organic compounds where the peaks are present but not all the information is concentrated around them). The peaks in this spectrum are located at the points 136.42, 129.63, 125.85, 19.66 ppm. This information has been obtained from the data base <http://sdbs.db.aist.go.jp>, (National Institute of Advanced Industrial Science and Technology, date of access August 23, 2015). Now, we might want to consider the ^{13}C -NMR spectrum of another closely related compound, the m-xylene, an isomer of the previous one: see the right panel of Figure 1. Although the general aspect of both spectra is very similar, there are clearly some differences. In the case of m-xylene, the peaks are located at 137.74, 129.96, 128.21, 126.13, 21.31 ppm. A “reasonable” metric defined to measure the distance between these graphics should provide a small value (thus reflecting their close affinity), by taking into account their “visual” proximity, that is, the distance between the graphics in all directions (not only in the vertical one). Moreover, for this type of graphics, we would also like to detect the presence of additional very narrow peaks (far away from the others), contributing a small area but carrying a relevant information on the compound. The d_2 distance does not seem useful for such purpose. See also the Figure 2 below and the discussion following definition (1).

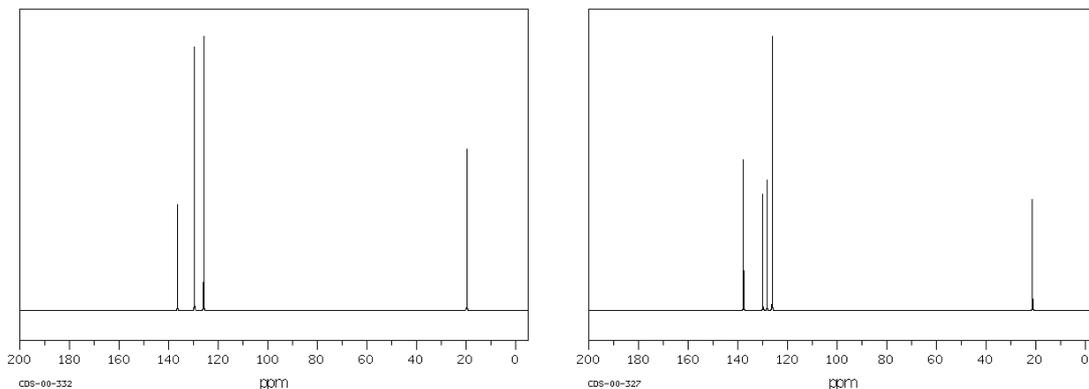


Figure 1: ^{13}C -NMR spectra of the o-xylene (left) and m-xylene.

As explained in depth by Coombes et al. (2007), in order to reach meaningful conclusions, handling of spectrum data needs a crucial pre-processing stage. This typically includes, among others, the following steps: *remove random noise*, *normalization*, *peaks detection* (to identify locations on the scale that correspond to specific molecules) and *peak matching* (to match

peaks in different samples, that correspond to the same peak). For this purpose, there is an increasing amount of software available. In particular, several packages can be downloaded from the web page of the software R (<http://www.r-project.org/>) in order to deal with spectrum-type data; for example, MALDIquant, readMzXmlData and aLFQ. This paper could be seen as a further suggestion in this line of research.

The rest of this paper is organized as follows: the study of the proposed visual metric (including the definition, computation and topological properties of the distance) is considered in Section 2. In Section 3 we focus on some theoretical aspects of the use of this metric in the supervised classification problem. A small simulation study is provided in Section 4. Two real data examples of mass spectra classification are considered in Section 5. Finally, some concluding remarks are given in Section 6. The proofs are given in an appendix.

2 A visual, Hausdorff-based distance for non-negative functions

The starting point is the standard definition (see, e.g., Rockafellar and Wets (2009), p. 117) of the Hausdorff (or Pompeiu-Hausdorff) distance between two compact non-empty sets, $A, C \subset \mathbb{R}^d$:

$$\begin{aligned} d_H(A, C) &= \inf\{\epsilon > 0 : A \subset B(C, \epsilon), C \subset B(A, \epsilon)\} \\ &= \max\left\{\max_{a \in A} d(a, C), \max_{c \in C} d(c, A)\right\}, \end{aligned}$$

where $B(A, \epsilon)$ denotes the ϵ -parallel set $B(A, \epsilon) = \cup_{x \in A} B(x, \epsilon)$ and $B(x, \epsilon)$ denotes (with a slight notational abuse) the closed ball centered at x with radius ϵ ; the open ball will be denoted $\overset{\circ}{B}(x, \epsilon)$. Also, $d(a, C) = \inf\{\|a - c\| : c \in C\}$.

Unlike other notions of proximity between sets, d_H is a true metric (i.e. it has the properties of identifiability, symmetry and triangular inequality) in the class of compact non-empty sets. The Hausdorff distance has been extensively used in different problems of image analysis (especially in pattern recognition), which appear in the literature under different names (shape comparison, object matching, etc.). The strong intuitive motivation behind the definition of d_H has motivated the study of other variants of the same idea as well as other closely associated notions. Some references are Huttenlocher et al. (1993), Dubuisson and Jain (1994), Sim et al. (1999).

However, our aim here is rather to use the Hausdorff metric as a tool for defining distance between functions, very much in the spirit of some ideas in approximation theory; see, for example, Sendov (1990).

The basic idea behind the metric we are going to consider is quite simple: given two non-negative functions f and g , defined on $[0, 1]$, the distance between f and g is measured in terms of the Hausdorff metric between the corresponding hypographs. However, we must take care of some technical aspects in order to properly establish this definition.

Let us recall that a function $f : [0, 1] \rightarrow \mathbb{R}$ is said to be *upper semicontinuous at x_0* if $\limsup_{x \rightarrow x_0} f(x) \leq f(x_0)$. A function f is said to be upper semicontinuous (USC) if it fulfils the above condition at every point x_0 .

Given a non-negative function f defined on $[0, 1]$, the *hypograph of f* is the set

$$H_f = \{(x, y) \in \mathbb{R}^2 : x \in [0, 1], 0 \leq y \leq f(x)\}.$$

Denote by \mathcal{E} the space of non-negative USC functions defined on $[0, 1]$. The following proposition, whose proof can be found in Natanson (1960), establishes some useful properties of USC functions.

Proposition 1. *Let $f : [0, 1] \rightarrow \mathbb{R}$ be a non-negative USC function.*

- 1) *Let $K \subset [0, 1]$ be a compact set. Then, there exists $z \in K$ such that $\sup_{x \in K} f(x) = f(z)$.*
- 2) *The hypograph H_f is compact.*

We are now ready to define our visual metric: for $f, g \in \mathcal{E}$ we define

$$\mathbb{H}(f, g) = d_H(H_f, H_g). \tag{1}$$

It is easily seen that this is a true metric in \mathcal{E} . In particular, if $d_H(H_f, H_g) = 0$, the USC assumption guarantees that we must have $f = g$.

Let us denote by $(\mathcal{E}, \mathbb{H})$ the space of USC non-negative functions endowed with the metric (1).

Figure 2 aims at illustrating the heuristic meaning of the \mathbb{H} -metric between two spectrum-type curves f_1 (solid line) and f_2 (dotted line). In this case, the distance $\mathbb{H}(f_1, f_2) = 0.077$ is the length of the double arrow joining two close peaks in the curves. The corresponding values for the “classical” distances are $d_\infty(f_1, f_2) = 0.952$, $d_2(f_1, f_2) = 0.119$. So, \mathbb{H} succeeds in reflecting the visual proximity between both curves.

Remark 1. *In order to gain some additional insight on the meaning of the distance \mathbb{H} and their relations with other usual metrics, let us note that*

- (a) *Convergence in \mathbb{H} does not imply pointwise convergence. Consider $f(x) = \mathbb{1}_{[0,1]}(x)$ and the sequence $f_n(x) = nx$ if $x < 1/n$ and $f_n(x) = 1$ if $x \in [1/n, 1]$. It is clear that $\mathbb{H}(f_n, f) \rightarrow 0$ but $f_n(0) \not\rightarrow f(0)$. The*

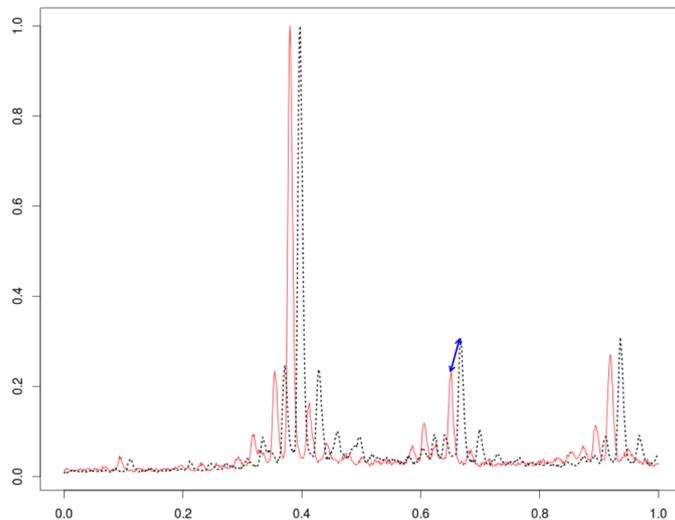


Figure 2: $\mathbb{H}(f_1, f_2)$ corresponds to the length of the double arrow joining both curves.

reciprocal implication is not true either. Take $f(x) = 0 \forall x \in [0, 1]$ and $f_n(x) = x^n(1 - x^n)$. We have $f_n(x) \rightarrow 0$ for all x but $\mathbb{H}(f_n, f_0) \rightarrow 0$ where $f_0(1) = 1/4$ and $f_0(x) = 0$ for $x \in [0, 1)$.

- (b) Convergence in L^p does not imply convergence in \mathbb{H} : consider $f_n(x) = \mathbb{I}_{[0, 1/n]}$ and $f(x) = 0 \forall x \in [0, 1]$. The reciprocal is also false: take $I_i^n(x) = \mathbb{I}_{[\frac{i-1}{2^n}, \frac{i}{2^n}]}(x)$ $i = 1, \dots, 2^n$, and the functions

$$f_n(x) = \sum_{k=1}^{2^n-2} I_{2k}^n(x) \quad \text{and} \quad f(x) = \mathbb{I}_{[0, 1]}(x),$$

it is clear that $\mathbb{H}(f, f_n) = 1/2^{n+1}$, however, for all p , $\int_0^1 |f_n(x) - f(x)|^p dx = 1/2$.

- (c) A natural question is: why to use USC functions? Since in many applications, the functional data appear as continuous functions, one might think that we might restrict our discussion to the continuous case. However there are, at least, good reasons for considering USC functions: first, in some practical examples (though not, typically, in the case of spectra) one has to deal with non-continuous samples and, especially, with jump discontinuities. Second, we need upper semicontinuity to

get a complete space (which in turn is essential for a more convenient mathematical handling). Take for example the sequence of functions $f_n(x) = x^n$ for $x \in [0, 1]$. This is a Cauchy sequence in our space $(\mathcal{E}, \mathbb{H})$, but clearly does not converge to any continuous function on $[0, 1]$. Hence, we need to enlarge the space to include USC if we want to get completeness.

2.1 Computational aspects

As mentioned above, the Hausdorff distance has some applications in image processing. Hence its numerical calculation has motivated some interest in the literature. See Nutanong et al. (2011) and Alt et al. (2003), just to mention a couple of recent references. The `Matlab` function `HausdorffDist` computes the Hausdorff distance between two finite sets of points in \mathbb{R}^2 . We are concerned here with the particular case in which the sets are the hypographs of functions, especially when these functions are specified only by their values in a given grid of $[0, 1]$. Our aim here is to approximate the value of $\mathbb{H}(f, g)$ in such cases, which arise very often in practical applications. First let us observe that, given two functions f and g in \mathcal{E} , from the definitions of \mathbb{H} and d_H we have: $\mathbb{H}(f, g) \leq d_H(\partial H_f, \partial H_g)$. However, the boundaries ∂H_f and ∂H_g do play a relevant role in the calculation of $\mathbb{H}(f, g)$. In fact, the following proposition shows that we can restrict the calculation to appropriate subsets of these boundaries.

Proposition 2. *Let $f, g \in \mathcal{E}$, then*

$$\mathbb{H}(f, g) = \max \left\{ \sup_{\substack{x=(x_1, x_2) \in \partial H_g \\ g(x_1) \geq f(x_1)}} d(x, \partial H_f), \sup_{\substack{y=(y_1, y_2) \in \partial H_f \\ f(y_1) > g(y_1)}} d(y, \partial H_g) \right\}.$$

The proofs of all results are given in the Appendix. In particular, the proof of Proposition 2, will require Lemma **A1** whose proof can also be found in the Appendix.

An algorithm to compute \mathbb{H}

If we have $\alpha_n^f = (t_1, f(t_1)), \dots, (t_n, f(t_n))$ and $\alpha_n^g = (t_1, g(t_1)), \dots, (t_n, g(t_n))$, and if we assume that f and g are continuous, then Proposition 2, together with Proposition **A1** in the Appendix, gives us a simple algorithm of order n^2 to approximate $\mathbb{H}(f, g)$. Just compute

$$\tilde{\mathbb{H}}(f, g) = \max \left\{ \max_{\{i: g(t_i) > f(t_i)\}} d((t_i, g(t_i)), \alpha_n^f), \max_{\{i: f(t_i) > g(t_i)\}} d((t_i, f(t_i)), \alpha_n^g) \right\},$$

where, if $\{i : g(t_i) > f(t_i)\} = \emptyset$ then $\max_{\{i:g(t_i)>f(t_i)\}} d((t_i, g(t_i)), \alpha_n^f) = 0$ and if $\{i : f(t_i) > g(t_i)\} = \emptyset$, then $\max_{\{i:f(t_i)>g(t_i)\}} d((t_i, f(t_i)), \alpha_n^g) = 0$. From Lemma **A1**, if $\max_i |t_{i+1} - t_i| \rightarrow 0$ then $\mathbb{H}(f, g) \rightarrow \mathbb{H}(f, g)$.

2.2 Some related literature

The distance \mathbb{H} has been considered in Cuevas and Fraiman (1998) in the context of density estimation: in particular, convergence rates are obtained, under some smoothness conditions, for $\mathbb{H}(\hat{f}_n, f)$, where \hat{f}_n denotes a sequence of kernel density estimators of the density f .

Different versions of the same idea are considered in Rockafellar and Wets (2009), p. 282. They are defined in terms of epigraphs (rather than hypographs) and are therefore applied to lower semicontinuous (rather than upper semicontinuous) functions. Some relevant applications are given in the framework of optimization theory to give bounds for approximately optimal solutions of convex lower semicontinuous functions.

Another related approach to the idea of defining the distance between two functions in terms of the distance between their graphs is considered in Sendov (1990) for the so-called *segment functions*. Holá (1992) extends these ideas to the setting of multifunctions.

2.3 Topological properties of $(\mathcal{E}, \mathbb{H})$

The metric space is particularly “well-behaving” in some important aspects that are summarized next.

Theorem 1. (a) *The space $(\mathcal{E}, \mathbb{H})$ is complete and separable. Also, any bounded and closed set in $(\mathcal{E}, \mathbb{H})$ is compact. In particular, $(\mathcal{E}, \mathbb{H})$ is locally compact.*

(b) *Let $f_n, f \in \mathcal{E}$ such that $\mathbb{H}(f_n, f) \rightarrow 0$ then;*

$$\max_{x \in [0,1]} f(x) = \lim_{n \rightarrow +\infty} \max_{x \in [0,1]} f_n(x).$$

The proof of this result is given in the Appendix. Let us now briefly comment on the meaning and usefulness of these properties.

- (i) Among the three properties established in Theorem 1 (a), completeness is perhaps the most basic one. It is essential to study convergence of sequences or series in $(\mathcal{E}, \mathbb{H})$ by just looking at the corresponding Cauchy property. This property is also required in the proof of some key results as Banach’s fixed point theorem for contraction mappings; see Grandas and Dugudji (2003)

- (ii) Separability is a most crucial property in a metric space in order to define on it well-behaving probability measures. A nice discussion on this topic can be found in Ledoux and Talagrand (1991), pp. 38-39. Although this discussion applies, in principle, to Banach spaces, the main arguments can be also translated to a metric space. For example, separability is required to ensure that a probability measure P defined on $(\mathcal{E}, \mathbb{H})$ is *tight*, in the sense that for all $\epsilon > 0$ there exists a compact set $K \subset \mathcal{E}$ such that $P(K) > 1 - \epsilon$. This is a far-reaching property, that can be found in the basis of many standard probability calculations. Thus, the separability property allows us to express any \mathcal{E} -valued random element as a limit of a sequence of simple (finite-valued) random elements. Also, separability is needed to guarantee a proper behaviour of product measurable structures: in particular, the Borel σ -algebra of the product space is the product of the individual Borel σ -algebras of the factors; see Proposition 1.5 in Folland (1999). Also, let us recall that separability of a metric space is equivalent to the property that this space is second-countable (e.g., Folland (1999), pp. 116-118), which is important in many probability arguments: for example, to show that any probability measure in a locally compact metric space is a Radon measure, see Folland (1999), Th. 7.8.

Finally, separability is also required for the consistency theorem for k -NN classification rules mentioned in Subsection 3.

- (iii) As for local compactness, let us recall that, in the case of Banach spaces, this property is equivalent to the finite-dimensionality of the space. In our case, we don't have a vector structure, so that we only have a metric space (not a normed one). However, the local compactness allows us to use some "natural" properties that we often use in the finite-dimensional spaces. For example, to show that any real integrable function defined on \mathcal{E} can be approximated by a sequence of continuous compact-supported functions (see Folland (1999), Proposition 7.9). An application of this can be found in Section 3.

Remark 2. *Let us observe that the local compactness does not hold for $(\mathcal{E}, \|\cdot\|_\infty)$. In order to see this, observe that for every $\epsilon > 0$, the sequence $f_n(x) = \epsilon x^n$ is included in the ball (with the distance $\|\cdot\|_\infty$) centered at the null function, of radius ϵ . However, this sequence does not have any convergent subsequence; indeed, the only possible limit would be the function $f_0(x) = 0$ for $x \in [0, 1)$, $f_0(1) = \epsilon$, but $\|f_n - f_0\|_\infty = \epsilon$ for all n .*

3 Applications to classification of functional data

We will briefly consider here some theoretical aspects of the supervised classification problem, focusing especially on the case of k -NN (nearest neighbors) classifiers.

The (functional) supervised classification problem

We focus on the problem of supervised classification with functional data; see e.g., Baíllo et al. (2011a) for an overview. More precisely, we are concerned with statistical problems for which the available data consist of an iid “training sample” $D_n = ((X_1, Y_1), \dots, (X_n, Y_n))$. The $X_i = \{X_i(t) : t \in [0, 1]\}$ are independent trajectories, belonging to a function space \mathcal{X} , drawn from a stochastic process $X := \{X(t) : t \in [0, 1]\}$ which can be observed from two probability distributions, P_0 and P_1 (often referred to as “populations” in statistical language). The Y_i are binary random variables indicating the membership of the trajectory X_i to P_0 or P_1 , that is, the population from which the observation X_i has been drawn. It is assumed that the conditional distributions of $X|Y = i$, $i = 0, 1$ (that is, P_0 and P_1) are different.

k -NN classifiers: why to use them in the functional setting

In a model of this type, the aim is typically to classify (either in P_0 or in P_1) a new observation X , for which the corresponding value of Y is unknown. A classification rule (or classifier) is a measurable function $g : \mathcal{X} \rightarrow \{0, 1\}$ defined on the space \mathcal{X} of trajectories. Usually, the classification rules are constructed using the information provided by the training sample data (X_i, Y_i) .

In this work we will limit ourselves to use the k -NN classifiers: an observation x is classified into P_0 if the majority among the k observations X_i (in the training sample) closest to x , fulfils $Y_i = 0$; ties are randomly broken. Of course, “closest” refer to some metric defined in the space \mathcal{X} on which the X_i take values: each metric leads to a different k -NN classification rule. In the functional infinite dimensional case, the choice of this metric is particularly relevant. The values $k = k_n$ are the smoothing parameters, similar to others which appear in non-parametric procedures: see Devroye et al. (1996) for background. As we will see below, they must fulfil some minimal conditions regarding the speed of convergence to infinity. Of course, the choice of k for any specific sample size n can have some influence on the performance of the k -NN classifier. However, as we will see in Section 5, the choice of the metric in the “feature space” (where X takes values) can be even more important.

The reasons for choosing k -NN classifiers can be summarized in the following terms: simplicity, ease of interpretability, good general performance

and generality. Indeed, k -NN is a sort of all-purposes “benchmark procedure”, not so easy to beat in practice. The available experience (see Baïllo et al. (2011, 2011a), Galeano et al. (2014) and references therein) suggests that, k -NN classifiers tend to show a stable performance, not far from the best method found in every specific problem. Moreover, they have a sound intuitive basis, so they are easily interpretable in all cases (unlike other classification methods) and they can be used in very general settings, when X takes values in any metric space. We now consider some theoretical issues regarding consistency of k -NN classifiers in the framework of our space $(\mathcal{E}, \mathbb{H})$.

The notion of consistency

Let us denote by g_n a sequence of k -NN classifiers defined in the usual way, as indicated at the end of the previous subsection. We will say that this sequence is *weakly consistent* (see, e.g., Devroye et al. (1996) for more details) if the misclassification probability $L_n = \mathbb{P}(g_n(X) \neq Y|D_n)$ converges (in probability, as $n \rightarrow \infty$) to the optimal value $L^* = \mathbb{P}(g^*(X) \neq Y)$, which corresponds to the optimal rule $g^*(x) = \mathbb{I}_{\{\eta(x) > 1/2\}}$, where $\eta(x) = \mathbb{E}(Y|X = x) = \mathbb{P}(Y = 1|X = x)$. It is readily seen that the weak consistency condition is equivalent to

$$\mathbb{E}(L_n) \longrightarrow \mathbb{E}(L^*).$$

In the finite dimensional case, that is when random variable X takes values in \mathbb{R}^d , it is well-known from a classical result due to Stone (1977), that any sequence of k -NN classifiers is (weakly) consistent provided that $k \rightarrow \infty$ and $k/n \rightarrow 0$. This result is *universal*, in the sense that it does not impose any condition of the distribution of the random pair (X, Y) .

The infinite-dimensional case. The Besicovitch condition

Let (X, Y) be the random element generating the data in a supervised functional classification problem, where X is \mathcal{E} -valued and Y takes values in $\{0, 1\}$. Denote by μ the distribution of X , $\mu(E) = \mathbb{P}(X \in E)$.

It is natural to ask whether the above mentioned universal consistency of the finite-dimensional k -NN classifiers still holds for the functional (infinite-dimensional) case. The answer is negative. There is, however, an additional technical condition which (together with $k \rightarrow \infty$, $k/n \rightarrow 0$), ensures weak consistency for the k -NN functional classifiers. While this condition is not in general trivial to check, it always holds whenever the regression function $\eta(x) = \mathbb{E}(Y|X = x)$ is continuous. The corresponding theory has been first developed by Cérou and Guyader (2006). In particular, the mentioned sufficient condition for consistency established by these authors is the following differentiability-type assumption (on the distribution of (X, Y)), called *Besi-*

covitch condition:

$$\lim_{\delta \rightarrow 0} \frac{1}{\mu(B(X, \delta))} \int_{B(X, \delta)} |\eta(X) - \eta(x)| d\mu(x) = 0, \text{ in probability.} \quad (2)$$

Here, $B(X, \delta)$ denotes the closed δ -ball centered at $X = X(t)$ in the space of trajectories of the process $X = X(t)$. A weaker, slightly simpler version of this property, almost identical to the conclusion of Lebesgue differentiation theorem, would be as follows,

$$\lim_{\delta \rightarrow 0} \frac{1}{\mu(B(X, \delta))} \int_{B(X, \delta)} \eta(x) d\mu(x) = \eta(X), \text{ in probability.} \quad (3)$$

Conditions (2) and (3) are clearly reminiscent of the conclusion of the classical Lebesgue Differentiation Theorem (see (Folland, 1999, p. 98)). Clearly (2) implies (3). It can be also seen that the μ -a.s. continuity of η is a sufficient condition for (2).

As mentioned above, Cérou and Guyader (2006, Th. 2) have proved that condition (2) together with $k \rightarrow \infty$ and $k/n \rightarrow 0$, ensures the weak consistency of a sequence of k -NN classifiers when X takes values in a separable metric space. On the other hand, Abraham et al. (2006) have used (3) as a sufficient condition for the consistency of kernel classification rules. They also need some supplementary conditions on the sequence $h = h_n$ of smoothing parameters and the space \mathcal{E} : they require that the existence of a sequence of non-decreasing totally bounded subsets, $\mathcal{F}_k \subset \mathcal{E}$, such that $\mu(\cup_k \mathcal{F}_k) = 1$ and a condition that relates the bandwidth h with the metric entropy of the subsets \mathcal{F}_k .

The following result shows that, in our case, the consistency holds for a class of “regular” distributions which is dense in the space of all distributions. In other words, the result shows that the assumption of continuity for the regression function $\eta(x)$ (which guarantees consistency for k -NN classifiers) is in fact not very restrictive, as any possible distribution for (X, Y) may be arbitrarily approximated by another one which fulfils this continuity condition.

Proposition 3. *Let us consider a binary supervised classification problem based on observations from (X, Y) , where X is \mathcal{E} -valued and Y is the binary variable indicating the class (0 or 1). Let g_n be a sequence of k -NN classifiers such that $k \rightarrow \infty$ and $k/n \rightarrow 0$.*

Whatever the distribution Q of (X, Y) there is another distribution P , arbitrarily close to Q in the weak topology, under which the regression function $\eta(x) = \mathbb{P}(Y = 1|X = x)$ is continuous with compact support and the sequence g_n is weakly consistent.

4 Some simulations

A simulation experiment has been carried out to illustrate a simple situation in which our “visual distance” could be especially suitable. The underlying model is very simple: the functional data are just “corrupted” trajectories of the absolute value of a Brownian Bridge (absBB) on $[0, 1]$. In the population P_0 the absBB trajectories are perturbed by just adding to them a spiky function identically null on $[0, 1]$ except for a triangular peak with basis 0.04 and height 1, whose center is randomly chosen on the interval $[0, a_1]$ for some $a_1 \leq 1/2$. The trajectories from P_1 are similarly constructed except that the center of the noise peak is randomly selected on $[a_2, 1]$ for some $1/2 \leq a_2 \leq 1$.

We have performed this experiment for two choices of (a_1, a_2) . The first case (Model 1, Table 4 left) corresponds to the choice $a_1 = a_2 = 1/2$. In the second one (Model 2, Table 4 right), we have taken $a_1 = 1/3, a_2 = 2/3$.

Figure 3 shows two trajectories drawn from Model 1, (in solid line, the trajectory drawn from P_0).

In both examples the training samples are of size 100 (50 trajectories drawn from each population). The outputs of the tables correspond to the average missclassification proportions (over 500 trajectories) of test samples of size 100 (50 generated from each population). The trajectories are discretized on a grid of 100 equispaced points.

As for the choice of k , we have checked a reasonable range (according to the sample size) of values, in order to check “robustness” with respect to k . We limit ourselves to odd values of k , from 3 to 9, just to avoid ties in the classifier output.

k	\mathbb{H}	d_2	d_∞
3	.144	.454	.363
5	.188	.486	.450
7	.222	.496	.483
9	.249	.499	.494

k	\mathbb{H}	d_2	d_∞
3	.031	.421	.275
5	.046	.473	.396
7	.062	.491	.459
9	.077	.497	.485

Table 1: Misclassification rates over 500 replications for different values of k under Model 1 (left panel) and Model 2 (right).

The results are self-explanatory: the classical distances have almost no discriminatory power in this example. The narrow noisy peaks are not suitable for them. This is in sharp contrast with the much better performance of the \mathbb{H} -distance.

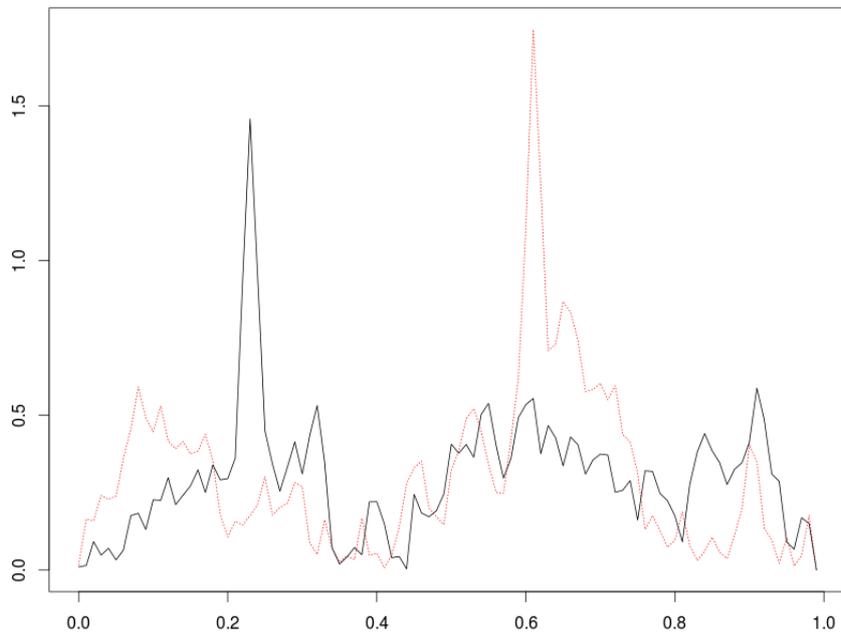


Figure 3: Two random trajectories drawn from Model 1: in solid line under P_0 , in dashed line under P_1 .

5 Real data examples

We will consider here two examples of binary classification based on functional data corresponding to mass spectra. The ovarian cancer data is a bio-medical example. Hence the samples drawn from P_0 and P_1 correspond, respectively, to a control, “healthy” group and to a “patients group”; the aim is to assign a new coming individual with spectrum x to one of these groups. The second example concerns food science: the goal is to investigate the capacity of mass spectra in order to discriminate between two varieties of coffee beans.

In both cases we have performed a similar experiment: the cross-validation (leave-one-out) proportions of correct classification have been computed for k -NN classifiers based on three different distances: the L^2 -metric, d_2 , the supremum metric d_∞ and our Hausdorff-based distance \mathbb{H} .

The main goal of this study is just to check the possible usefulness of the “visual” distance \mathbb{H} when compared with the classical choices d_2 and d_∞ . In principle, the idea was to handle the functional data themselves

(or rather their available discretized versions) avoiding the use of dimension reduction techniques via linear projections (principal components, partial least squares) or variable selection methods. In these examples, the available sample sizes are quite modest (especially in the second one). So the results must be interpreted with caution, just as useful hints of the performance of our proposal in real data problems. Obviously more research is needed.

5.1 The ovarian cancer data

These data correspond to mass spectra from blood samples of 216 women: 95 belong to the control group (CG) and the remaining 121 suffer from an ovarian cancer condition (OC). The use of mass spectra as a diagnostic tool in this situation is based on the fact that some proteins produced by cancer cells tend to be different (either in amount or in type) from that of the normal cells. These differences could be hopefully detected via mass spectrometry. We refer to Banks and Petricoin (2003) for a previous analysis of these data with a detailed discussion of their medical aspects. See also Cuesta-Albertos et. al. (2006) for further statistical analysis of these data. The raw data were defined on finite grids (of sizes varying between 320.000 and 360.000) on the interval $[700, 12000]$. In order to facilitate the computational treatment we did some pre-processing: first, we have restricted ourselves to the interval mass charge $[7000, 9500]$, where most peaks were concentrated. Second, we denoised the data by defining the spectra as 0 at those points for which the value was smaller than 5 (this value was chosen after trying with several others). Third, in order to have all the spectra defined in a common equispaced grid (we took a grid of size 20001), we have smoothed them via a Nadaraya-Watson procedure. Finally, every function has been divided by its maximum, in order to have all the values scaled in the common interval $[0, 1]$. This amounts to assume that the location of the peaks are important, but not the corresponding heights.

The results of our analysis are shown in Table 2 below.

k	\mathbb{H}	d_2	d_∞
3	.125	.092	.125
5	.079	.092	.116
7	.083	.088	.125
9	.143	.111	.143

Table 2: Classification error rates for the ovarian cancer data using k -NN classifiers based on three different distances.

We have kept the same values of k considered in the simulation study. It can be seen that in all cases the "optimum" is either $k = 5$ or $k = 7$ and, for these choices, the Hausdorff based distance clearly outperforms the other two metrics d_2 and d_∞ .

5.2 The coffee data

These data consist of 28 mass spectra (discretized in a grid of 286 values) corresponding to coffee beans of two varieties, *Arabica* and *Robusta*. The respective sample sizes are 15 and 13. These data are available from the web page http://www.cs.ucr.edu/~eamonn/time_series_data/ of the University of California, Riverside. In this case the pre-processing consisted only on a rescaling of both axes to fit the data on $[0, 1]^2$.

k	\mathbb{H}	d_2	d_∞
3	.071	.071	.036
5	.036	.179	0
7	.107	.214	.036
9	.071	.25	.036

Table 3: Classification error rates for the coffee data using k -NN classifiers based on three different distances.

In this case the \mathbb{H} -based classifiers are outperformed by those based on the supremum distance d_∞ but are clearly better than those based on d_2 . It is curious to note the unstable behavior of d_2 , which is almost competitive in the cancer example but gets the worst performance both in the simulation study and in the coffee data example. On the other hand, d_∞ ranked clearly the last one in the cancer example. The \mathbb{H} -based methodology is never the worst one in the considered examples. Again, more detailed experiments are needed to confirm or refute this provisory findings.

6 Concluding remarks

The choice of a distance is particularly relevant when dealing with functional data. Not only some classifiers (as those of k -NN type or others based on depth measures) are defined in terms of distances, but also the theoretical properties (regarding consistency, convergence rates or asymptotic distributions) must be necessarily established in terms of a given distance in the sample space. Of course, in the finite-dimensional case, the use of different

norms in the Euclidean sample space can lead to different results in a classification problem. However, the case for considering different norms in this finite-dimensional situation is not very strong, due to the well-known fact that all the norms are equivalent in finite-dimensional normed spaces.

Our generic suggestion here is to consider geometrically motivated distances in functional data. The specific proposal we make, $\mathbb{H}(f, g)$ is just one possibility; several other alternatives might be considered. The book by Rockafellar and Wets (2009) could suggest some ideas in this regard. While our theoretical and practical results with the distance \mathbb{H} are encouraging, it is also quite clear that this metric suffers from some limitations: first, we are restricted to non-negative functions. Second, the extension of this idea to functions of several variables would probably involve considerable computational difficulties. Third, much more theoretical development is needed; in particular, the study of probability measures on the space $(\mathcal{E}, \mathbb{H})$ is essential if we want to use theoretical models combined with the distance \mathbb{H} . In fact, this need for a deeper mathematical development is a common feature for most chapters of the, still young, FDA theory.

Appendix

Proof of Proposition 2

To prove this Proposition we first must prove an auxiliary result:

Lemma A1. *If $f, g \in \mathcal{E}$, then there exist $u \in \partial H_f$ and $v \in \partial H_g$ such that*

$$\mathbb{H}(f, g) = d(u, H_g) = d(v, H_f) = \|u - v\|. \quad (4)$$

Proof. We have, by definition of \mathbb{H} :

$$\mathbb{H}(f, g) = d_H(H_f, H_g) = \max \left\{ \sup_{a \in H_f} d(a, H_g), \sup_{b \in H_g} d(b, H_f) \right\}.$$

Assume $\mathbb{H}(f, g) > 0$. Otherwise the result is trivial. Let us suppose by contradiction that there is no pair $(u, v) \in \partial H_f \times \partial H_g$ such that (4) is fulfilled. In any case, the compactness of H_f and H_g guarantees the existence of $x = (x_1, x_2)$ and $y = (y_1, y_2)$ fulfilling (4) but, according to our contradiction argument, either x or y must be an interior point. For example, if $x \in \text{int}(H_f)$, then $0 < x_1 < 1$. We will see that $d((x_1, f(x_1)), H_g) \geq \mathbb{H}(f, g)$. For every $t \in [0, 1]$ such that $|t - x_1| < \mathbb{H}(f, g)$ let us denote $u^t = (t, u_2^t)$ and $v^t = (t, v_2^t)$ the intersection points of $\partial B(x, \mathbb{H}(f, g))$ and the line $x_1 = t$; with $u_2^t < v_2^t$. From the assumption on x , $d(x, H_g) = \mathbb{H}(f, g)$. This entails that $\bar{B}(x, \mathbb{H}(f, g)) \cap H_g = \emptyset$ and, since H_g is a hypograph (which implies that if

$(a, b) \in H_g$ then the segment joining (a, b) and $(a, 0)$ is included in H_g it is clear that $g(t) \leq u_2^t$, for all $t \in [0, 1]$ with $|t - x_1| < \mathbb{H}(f, g)$. Therefore, if we move upwards the point $x = (x_1, x_2)$ to $(x_1, f(x_1))$ (recall that from the USC assumption, $x_2 \leq f(x_1)$), we have $\dot{B}((x_1, f(x_1)), \mathbb{H}(f, g)) \cap H_g = \emptyset$ and then $d((x_1, f(x_1)), H_g) \geq \mathbb{H}(f, g)$. We cannot have $d((x_1, f(x_1)), H_g) > \mathbb{H}(f, g)$ since $(x_1, f(x_1)) \in H_f$ and $\mathbb{H}(f, g) = d_H(H_f, H_g)$. So, we must have $d((x_1, f(x_1)), H_g) = \mathbb{H}(f, g)$ with $u := (x_1, f(x_1)) \in \partial H_f$. As a consequence, we must also have a point $v \in \partial H_g$ such that $\|u - v\| = \mathbb{H}(f, g)$. This contradicts the assumption we made about the non-existence of such a pair (u, v) . □

We now prove Proposition 2.

Proof. Let us denote

$$d = \max \left\{ \sup_{\substack{x=(x_1, x_2) \in \partial H_g \\ g(x_1) \geq f(x_1)}} d(x, \partial H_f), \sup_{\substack{y=(y_1, y_2) \in \partial H_f \\ f(y_1) > g(y_1)}} d(y, \partial H_g) \right\}.$$

The case $\mathbb{H}(f, g) = 0$ is trivial, so let us assume $\mathbb{H}(f, g) > 0$. We will first see that $\mathbb{H}(f, g) \leq d$. Since H_f and H_g are compact, there are two possibilities:

- 1) there exists $x \in H_g$ such that $\mathbb{H}(f, g) = d(x, \partial H_f)$, or
- 2) there exists $y \in H_f$ such that $\mathbb{H}(f, g) = d(y, \partial H_g)$.

Let us suppose that we are in the first case. By Lemma **A1** we can assume that $x = (x_1, x_2) \in \partial H_g$. Since $\mathbb{H}(f, g) > 0$ and H_f is a hypograph it must be $g(x_1) > f(x_1)$, then $x \in \{x = (x_1, x_2) \in \partial H_g : g(x_1) \geq f(x_1)\}$ from where it follows that $\mathbb{H}(f, g) \leq d$. If we are in case 2, again by Lemma **A1**, we can assume $y = (y_1, y_2) \in \partial H_f$, as $\mathbb{H}(f, g) > 0$ and H_g is a hypograph it must be $f(y_1) > g(y_1)$, then $y \in \{y = (y_1, y_2) \in \partial H_f : f(y_1) > g(y_1)\}$. from where it follows that $\mathbb{H}(f, g) \leq d$. The inequality $\mathbb{H}(f, g) \geq d$ follows directly from the definition of \mathbb{H} . □

We also use the following proposition in the algorithm to calculate $\mathbb{H}(f, g)$ for f and g continuous.

Proposition A1. *Let $f, g \in \mathcal{E}$ be continuous functions, let u and v be the points of Lemma **A1**. Then, there exist $t \in [0, 1]$ and $s \in [0, 1]$ such that $u = (t, f(t))$ and $v = (s, g(s))$.*

Proof. Again, assume $\mathbb{H}(f, g) > 0$. By Lemma **A1** $u \in \partial H_f$, $v \in \partial H_g$, and $\mathbb{H}(f, g) = \|u - v\|$. So it is enough to prove that $u = (t, f(t))$ and $v = (s, g(s))$. Since f is continuous and $u \in \partial H_f$, there are four possibilities: (and the same holds for $v \in \partial H_g$) :

1. u is in the left border: $u = (0, u_2)$ with $u_2 < f(0)$.
2. u is in the right border: $u = (1, u_2)$ with $u_2 < f(1)$.
3. u is in the lower border: $u = (u_1, 0)$ with $0 \leq u_1 \leq 1$.
4. u is in the upper border: $0 \leq u_1 \leq 1$ y $u_2 = f(u_1)$.

We now prove that u can only be in Case 4. It is clear that Case 3 is not possible because both functions are non-negative. Cases 1 and 2 are also excluded following the ideas used in Lemma **A1**. For example, let us suppose that we are in Case 1 (see Figure 4). First observe that $\mathring{B}((0, f(0)), \mathbb{H}(f, g)) \cap H_g = \emptyset$; otherwise there would exist $(t_1, t_2) \in \mathring{B}((0, f(0)), \mathbb{H}(f, g)) \cap H_g$, then, the segment joining the points $(t_1, 0)$ and (t_1, t_2) (which is included in H_g) intersects $\mathring{B}(u, \mathbb{H}(f, g))$. But this contradicts $\mathbb{H}(f, g) = d_H(H_f, H_g)$. So we conclude $d((0, f(0)), H_g) \geq \mathbb{H}(f, g)$. However $d((0, f(0)), H_g) > \mathbb{H}(f, g)$ leads to a contradiction with the definition of $\mathbb{H}(f, g)$. Also, $d(u, H_g) = d((0, f(0)), H_g)$ leads to another contradiction. Indeed, if this were the case, we would have two points $((0, u_2)$ and $(0, f(0)))$ on the vertical axis $x_1 = 0$ which are equidistant to the hypograph H_g . Then we have three possibilities:

- (a) $u_2 < g(0) < f(0)$. This contradicts $d(u, H_g) = d((0, f(0)), H_g)$, since all the points $(0, u_3)$ with $u_2 < u_3 < g(0)$ belong to H_g .
- (b) $g(0) \leq u_2$: this contradicts the continuity of g since H_g must have a point in the boundary of $B((0, f(0)), d((0, f(0)), H_g))$ and no point in the open ball $\mathring{B}((0, u_2), d((0, u_2), H_g))$.
- (c) $g(0) \geq f(0)$: this is not compatible with $d(u, H_g) = d((0, f(0)), H_g)$. \square

Proof of Theorem 1.

(a) To state the local compactness we will in fact prove a slightly stronger property: we will show that any closed and bounded set in $(\mathcal{E}, \mathbb{H})$ is compact. Indeed, this would imply that the closed balls are compact. Since the family of balls with center at a given point is a local base, the local compactness will follow.

Since we are in a metric space compactness is equivalent to sequential compactness. Let us take $\{f_n\} \subset \mathcal{E}$ a bounded sequence; we will prove that this sequence has necessarily a convergent subsequence. To see this,

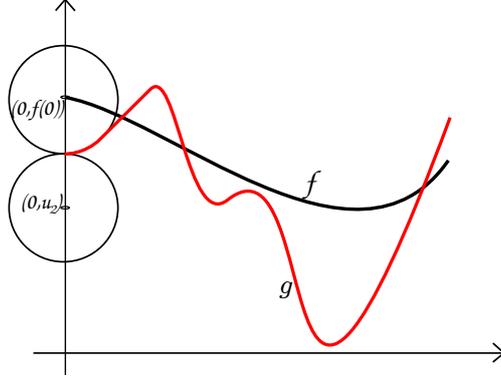


Figure 4: We cannot have $d(u, H_g) = d((0, f(0)), H_g)$ with $u = (0, u_2)$ and $u_2 < f(0)$.

note that the corresponding sequence of compact sets H_{f_n} is bounded. So it has convergent subsequence, which we may denote again by H_{f_n} , in the Hausdorff metric (since the closed and bounded sets are compact in the space of compact sets with the Hausdorff metric). Denote by C the limit of that subsequence. Therefore it is enough to prove that

if $\{H_{f_n}\}_n$ fulfils $H_{f_n} \rightarrow C$ for some compact set C , then there exists a USC function $f : [0, 1] \rightarrow [0, \infty)$, such that $C = H_f$. (5)

Let us take $(x, y) \in C$ and $(x_n, y_n) \in H_{f_n}$ converging to (x, y) ; note that there exists at least one such sequence because $d_H(H_{f_n}, C) \rightarrow 0$. Now, since the H_{f_n} are hypographs the vertical segment $[(x_n, 0), (x_n, y_n)]$ joining the points $(x_n, 0)$ and (x_n, y_n) is included in H_{f_n} . So $H_{f_n} \rightarrow C$, implies

$$\left[(x, 0), (x, \limsup f_n(x_n)) \right] \subset C. \quad (6)$$

Indeed, since H_{f_n} is a hypograph, $f_n(x_n) \geq y_n$. Then if we take \limsup we obtain $y \leq \limsup f_n(x_n)$ and $\{(x, z) : 0 \leq z \leq \limsup f_n(x_n)\} \subset C$.

Let us now define $f : [0, 1] \rightarrow [0, \infty)$ by

$$f(x) = \sup_{\{x_n\}:x_n \rightarrow x} \limsup f_n(x_n).$$

Since $\{f_n\}$ is bounded, f is well defined as a real-valued function. Let us prove that $C = H_f$. Since C is closed, we have, by (6), $H_f \subset C$. Moreover, if $(x, y) \in C$, taking $(x_n, y_n) \rightarrow (x, y)$ with $(x_n, y_n) \in H_{f_n}$, $f(x) \geq \limsup f_n(x_n) \geq \limsup y_n = y$, we obtain $(x, y) \in H_f$.

It remains to prove that f is USC. Suppose by contradiction that there exists $a \in [0, 1]$ such that $\limsup_{x \rightarrow a} f(x) > f(a)$. Then, we can take a

constant $\delta > 0$ and a sequence $x_n \rightarrow a$, $x_n \neq a$ for all n such that $f(x_n) > f(a) + \delta$ for n large enough, say $n > n_0$. By the definition of f , for every x_n we can take a sequence $z_n^k \rightarrow_k x_n$ (dependent on n), such that $f(x_n) = \lim_{z_n^k \rightarrow_k x_n} \limsup f_k(z_n^k)$.

Given $\varepsilon > 0$, for every $n > n_0$ let us take an increasing sequence $k(n) > n_0$ with

$$|z_n^{k(n)} - x_n| < \frac{1}{n} \text{ and } |f_{k(n)}(z_n^{k(n)}) - \limsup f_k(z_n^k)| < \varepsilon,$$

that is, $|f_{k(n)}(z_n^{k(n)}) - f(x_n)| < \varepsilon$. But as $z_n^{k(n)} \rightarrow_n a$ this contradicts $f(x_n) > f(a) + \delta$ for $n > n_0$.

Completeness follows directly from the fact that the space of compact sets endowed with the Hausdorff metric is complete, together with (5).

To prove separability, let \mathcal{P}_n be the set of all partitions of $[0, 1]$ defined by $0 = x_0 < x_1 < \dots < x_{n-1} < x_n = 1$ where the x_i are rational numbers. Denote $\mathcal{P} = \cup_n \mathcal{P}_n$. Note that \mathcal{P} is numerable.

Given a partition $\mathcal{P} \in \mathcal{P}_n$ and a set q_0, \dots, q_{n-1} of rational numbers, let us define

$$f_{\mathcal{P}}(x) = \begin{cases} q_0 & \text{if } x \in [0, x_1) \\ q_i & \text{if } x \in (x_i, x_{i+1}) \quad 1 \leq i \leq n-3 \\ q_{n-1} & \text{if } x \in (x_{n-1}, 1] \\ \max\{q_i, q_{i+1}\} & \text{if } x = x_i \quad 1 \leq i \leq n-2 \end{cases} \quad (7)$$

It is immediately seen that this function is USC and bounded. Let us see that the (numerable) set of all functions defined by 7, for all possible partitions \mathcal{P} and rational values q_i is dense in \mathcal{E} with respect to \mathbb{H} . Let f be a non-negative USC function and take $\varepsilon > 0$. Consider $\mathcal{P} \in \mathcal{P}_n$ a partition of the form $0 = x_0 < x_1 < \dots < x_{n-1} < x_n = 1$ where x_i are rational numbers and such that $\max_{i=0, \dots, n-1} |x_{i+1} - x_i| < \varepsilon/2$. By Proposition 1 there exists $f_i = \max_{x \in [x_i, x_{i+1}]} f(x)$. Let us take q_0, \dots, q_{n-1} rational numbers such that $q_i > f_i$ and $q_i - f_i < \varepsilon/2$ for all i . For this partition and this set of rational numbers let us define $f_{\mathcal{P}}$ as in (7). Now we claim that $\mathbb{H}(f_{\mathcal{P}}, f) \leq \varepsilon$. Indeed, it is clear that $f_{\mathcal{P}}(x) > f(x)$ for all $x \in [0, 1]$ so that $H_f \subset H_{f_{\mathcal{P}}}$, and $\mathbb{H}(f_{\mathcal{P}}, f) = \sup_{z \in H_{f_{\mathcal{P}}}} d(z, H_f)$. Given $z = (z_1, z_2) \in H_{f_{\mathcal{P}}}$, there exists $0 \leq i_0 \leq n-1$ such that $x_{i_0} \leq z_1 \leq x_{i_0+1}$. Now, choose t such that $x_{i_0} \leq t \leq x_{i_0+1}$ and $f_{i_0} = f(t)$. We have $z_2 < f(t) + \varepsilon/2$ and then $d(z, H_f) < \varepsilon$. Since z was an arbitrary point in $H_{f_{\mathcal{P}}}$ we finally get $\sup_{z \in H_{f_{\mathcal{P}}}} d(z, H_f) \leq \varepsilon$.

(b) By Proposition 1 (i) we know that there exists $z \in [0, 1]$ such that $f(z) = \max_{x \in [0, 1]} f(x)$. As $\mathbb{H}(f_n, f) \rightarrow 0$ there exist $x^n = (x_1^n, x_2^n) \in H_{f_n}$

such that $x_n \rightarrow (z, f(z))$. Then, $x_2^n \leq f_n(x_1^n) \leq \max_{x \in [0,1]} f_n(x)$ and, since $x_2^n \rightarrow f(z)$, we obtain

$$\max_{x \in [0,1]} f(x) = f(z) \leq \liminf_{n \rightarrow +\infty} \max_{x \in [0,1]} f_n(x) \leq \limsup_{n \rightarrow +\infty} \max_{x \in [0,1]} f_n(x).$$

Finally, let us prove that $\limsup_n \max_{x \in [0,1]} f_n(x) \leq \max_{x \in [0,1]} f(x)$. Denote $z_0 = \limsup_n \max_{x \in [0,1]} f_n(x)$. There exists $x_n \in [0, 1]$ such that $f_n(x_n) \rightarrow z_0$ with $f_n(x_n) = \max_{x \in [0,1]} f_n(x)$. Taking if necessary a subsequence, we can assume that $x_n \rightarrow x_0 \in [0, 1]$. Since $(x_0, z_0) \in H_f$ we have $f(x_0) \geq z_0$ then $\max_{x \in [0,1]} f(x) \geq z_0$.

Proof of Proposition 3.

Proof. This result is just a direct corollary from Th. 2 in Cérou and Guyader (2006) (recall that the continuity of $\eta(x)$ is a sufficient condition for (2)), combined with the fact that the regression function $\eta_Q(x) = \mathbb{P}(Y = 1|X = x)$ (i.e., the regression function under Q) can be approximated by a continuous compact supported function; we use here the local compactness of \mathcal{E} (see Folland (1999), Proposition 7.9). Indeed, note that the joint distribution of (X, Y) is completely determined by $\eta(x) = \mathbb{P}(Y = 1|X = x)$ and by the marginal distribution μ of X . Then, given Q , one can construct P by just approximating $\eta_Q(x) = \mathbb{P}(Y = 1|X = x)$ by a continuous compact-supported function $\eta_P(x)$ which, without loss of generality, can be taken $0 \leq \eta_P \leq 1$. Then, the distribution P determined by η_P and the marginal distribution μ of X is arbitrarily close to Q (just taking η_P close enough to η). Indeed, given any Borel set $C \subset \mathcal{E} \times \{0, 1\}$, consider the sets $C_0 = \{x \in \mathcal{E} : (x, 0) \in C\}$ and $C_1 = \{x \in \mathcal{E} : (x, 1) \in C\}$. Then,

$$Q(C) = \int_{C_0} (1 - \eta_Q(x)) d\mu(x) + \int_{C_1} \eta_Q(x) d\mu(x),$$

and

$$P(C) = \int_{C_0} (1 - \eta_P(x)) d\mu(x) + \int_{C_1} \eta_P(x) d\mu(x),$$

which can be made arbitrarily close. \square

Acknowledgements

A. Cuevas and R. Fraiman have been partially supported by Spanish Grant MTM2013-44045-P.

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