

# GENERALIZED DENSITY CLUSTERING<sup>1</sup>

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We study generalized density-based clustering in which sharply defined clusters such as clusters on lower-dimensional manifolds are allowed. We show that accurate clustering is possible even in high dimensions. We propose two data-based methods for choosing the bandwidth and we study the stability properties of density clusters. We show that a simple graph-based algorithm successfully approximates the high density clusters.

**1. Introduction.** It has been observed that classification methods can be very accurate in high-dimensional problems, apparently contradicting the curse of dimensionality. A plausible explanation for this phenomenon is the “low noise” condition described, for instance, in [Mammen and Tsybakov \(1999\)](#). When the low noise condition holds, the probability mass near the decision boundary is small and fast rates of convergence of the classification error are possible in high dimensions.

Similarly, clustering methods can be very accurate in high-dimensional problems. For example, clustering subjects based on gene profiles and clustering curves are both high-dimensional problems where several methods have worked well despite the high dimensionality. This suggests that it may be possible to find conditions that explains the success of clustering in high-dimensional problems.

In this paper, we focus on clusters that are defined as the connected components of high density regions [[Cuevas and Fraiman \(1997\)](#), [Hartigan \(1975\)](#)]. The advantage of density clustering over other methods is that there is a well-defined population quantity being estimated and density clustering allows the shape of the clusters to be very general. (A related but somewhat different approach for generally shaped clusters is spectral clustering; see [von Luxburg \(2007\)](#) and [[Ng, Jordan and Weiss \(2002\)](#)].) Of course, without some conditions, density estimation is subject to the usual curse of dimensionality. One would hope that an appropriate low noise condition would obviate the curse of dimensionality. Such assumptions have been proposed by [Polonik \(1995\)](#), [Rigollet \(2007\)](#), [Rigollet and Vert \(2006\)](#), and others. However, the assumptions used by these authors rule out the case where

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the clusters are very sharply defined, which should be the easiest cases, and, more generally, clusters defined on lower dimensional sets.

The purpose of this paper is to define a notion of density clusters that does not rule out the most favorable cases and is not limited to sets of full dimension. We study the risk properties of density-based clustering and its stability properties, and we provide data-based methods for choosing the smoothing parameters.

The following simple example helps to illustrate our motivation. We refer the reader to the next section for a more rigorous introduction. Suppose that a distribution  $P$  is a mixture of finitely many point masses at distinct points  $x_1, \dots, x_k$  where  $x_j \in \mathbb{R}^d$ . Specifically, suppose that  $P = k^{-1} \sum_{j=1}^k \delta_j$  where  $\delta_j$  is a point mass at  $x_j$ . The clusters are  $C_1 = \{x_1\}, \dots, C_k = \{x_k\}$ . This is a trivial clustering problem even if the dimension  $d$  is very high. The clusters could not be more sharply defined yet the density does not even exist in the usual sense. This makes it clear that common assumptions about the density such as smoothness or even boundedness are not well-suited for density clustering.

Now let  $p_h = dP_h/d\mu$  be the Lebesgue density of the measure  $P_h$  obtained by convolving  $P$  with the probability measure having Lebesgue density  $K_h$ , a kernel with bandwidth  $h$ . Unlike the original distribution  $P$ ,  $P_h$  has full-dimensional support for each positive  $h$ . The “mollified” density  $p_h$  contains all the information needed for clustering. Indeed, there exist constants  $\bar{h} > 0$  and  $\lambda \geq 0$  such that the following facts are true:

1. for all  $0 < h < \bar{h}$ , the level set  $\{x : p_h(x) \geq \lambda\}$  has disjoint, connected components  $C_1^h, \dots, C_k^h$ ;
2. the components  $C_j^h$  contain the true clusters:  $C_j \subset C_j^h$  for  $j = 1, \dots, k$ ;
3. although  $C_j^h$  overestimates the true cluster  $C_j$ , this overestimation is inconsequential since  $P(C_j^h - C_j) = 0$  and hence a new observation will not be misclustered;
4. let  $\hat{p}_h$  denote the kernel density estimator using  $K_h$  with fixed bandwidth  $0 < h < \bar{h}$  and based on a i.i.d. sample of size  $n$  from  $P$ . Then,  $\sup_x |p_h(x) - \hat{p}_h(x)| = O(\sqrt{\log n/n})$  almost everywhere  $P$ , which does not depend on the dimension  $d$  (see Section 3.1). The bias from using a fixed bandwidth  $h$ —which does not vanish as  $n \rightarrow \infty$ —does not adversely affect the clustering.

In summary, we can recover the true clusters using an estimator of the density  $p_h$  with a large bandwidth  $h$ . It is not necessary to assume that the true density is smooth or that it even exists.

Our contributions in this paper are the following:

1. We develop a notion of density clustering that applies to probability distributions that have nonsmooth Lebesgue densities or do not even admit a density.
2. We find the rates of convergence for estimators of these clusters.
3. We study two data-driven methods for choosing the bandwidth.

4. We study the stability properties of density clusters.
5. We show that the depth-first search algorithm on the  $\rho$ -nearest neighborhood graph of  $\{\widehat{\rho}_h \geq \lambda\}$  is effective at recovering the high-density clusters.

Another approach to clustering that does not require densities is the minimum volume set approach [Polonik (1995), Scott and Nowak (2006)]. Our approach is different because we are specifically trying to capture the idea that kernel density estimates are useful for clustering even when the density may not exist.

Section 2 contains notation and definitions. Section 3 contains results on rates of convergence. We give a data-driven method for choosing the bandwidth in Section 4. Section 4.2 contains results on cluster stability. The validity of the graph-based algorithm for approximating the clusters is proved in Section 5. Section 6 contains some examples based on simulated data. Concluding remarks are in Section 7. All proofs are in the Section 8. Some technical details are in the Appendix.

*Notation.* For two sequences  $\{a_n\}$  and  $\{b_n\}$ , we write  $a_n = O(b_n)$  and  $a_n = \Omega(b_n)$  if there exists a constant  $C > 0$  such that, for all  $n$  large enough,  $|a_n|/b_n \leq C$  and  $|a_n|/b_n \geq C$ , respectively. If  $a_n = \Omega(b_n)$  and  $a_n = O(b_n)$ , then we will write  $a_n \asymp b_n$ . We denote with  $\mathbb{P}(E)$  the probability of a generic event  $E$ , whenever the underlying probability measure is implicitly understood from the context. By the dimension of a Euclidean set, we will always mean the  $k$ -dimensional Hausdorff dimension for some integer  $0 \leq k \leq d$  (see the Appendix). These sets may consist, for example, of smooth submanifolds or even single points.

## 2. Settings and assumptions.

2.1. *Level set clusters.* In this section, we develop a probabilistic framework for the definition of clusters we have adopted. For ease of readability, the more technical measure-theoretic details are given in the Appendix.

Let  $P$  be a probability distribution on  $\mathbb{R}^d$  whose support  $S$  (the smallest closed set of  $P$ -measure 1) is comprised of an unknown number  $m$  of disjoint compact sets  $\{S_1, \dots, S_m\}$  of different dimensions. We define the *geometric density* of  $P$  as the measurable function  $p: \mathbb{R}^d \mapsto \mathbb{R}$  given by

$$(1) \quad p(x) = \lim_{h \downarrow 0} \frac{P(B(x, h))}{v_d h^d},$$

where  $B(x, \varepsilon)$  is the Euclidean ball of radius  $h$  centered at  $x$ ,  $\mu$  is the  $d$ -dimensional Lebesgue measure and  $v_d \equiv \mu(B(0, 1))$ . Note that, almost everywhere  $P$ ,  $p(x) = \infty$  if and only if  $x$  belongs to some set  $S_i$  having dimension strictly less than  $d$  and is positive and finite if and only if  $x$  belongs to some  $d$ -dimensional set  $S_i$ . In general,  $\int_{\mathbb{R}^d} p(x) d\mu(x) \leq 1$  and, therefore,  $p$  is not necessarily a probability density. Nonetheless,  $p$  can be used to recover the support of  $P$ , since

$$S = \overline{\{x : p(x) > 0\}},$$

where for a set  $A \subset \mathbb{R}^d$ ,  $\bar{A}$  denotes its closure.

For  $\lambda \geq 0$ , define the  $\lambda$ -level set

$$(2) \quad L \equiv L(\lambda) = \overline{\{x : p(x) \geq \lambda\}},$$

and its boundary  $\partial L(\lambda) = \{x : p(x) = \lambda\}$ . Throughout the paper, we will suppose that we are given a fixed value of  $\lambda < \|p\|_\infty$ , where  $\|p\|_\infty \equiv \sup_{x \in \mathbb{R}^d} p(x)$ . Often,  $\lambda$  is chosen so that  $P(L(\lambda)) \approx 1 - \alpha$  for some given  $\alpha$ . In practice, it is advisable to present the results for a variety of values of  $\lambda$  as we discuss in Section 7.

We assume that there are  $k \geq 1$  disjoint, compact, connected sets  $C_1(\lambda), \dots, C_k(\lambda)$  such that

$$L = C_1(\lambda) \cup \dots \cup C_k(\lambda).$$

We will often write  $C_j$  instead of  $C_j(\lambda)$  when the dependence of  $\lambda$  is clear from the context. The value of  $k$  is not assumed to be known. The sets  $C_1, \dots, C_k$  are called the  $\lambda$ -clusters of  $p$ , or just *clusters*. In our setting, the  $C_j$ 's need not be full dimensional. Indeed,  $C_j$  might be a lower-dimensional manifold or even a single point. Furthermore, if  $S_i$  has dimension smaller than  $d$ , then  $C_j = S_i$ , for some  $j = 1, \dots, k$ . Thus, for any  $\lambda \geq 0$ , the  $\lambda$ -clusters of  $p$  will include all the lower-dimensional components of  $S$ . On the other hand, if  $S_i$  is full-dimensional, then there may be multiple clusters in it, depending on the value of  $\lambda$ .

We observe an i.i.d. sample  $X = (X_1, \dots, X_n)$  from  $P$ , from which we construct the kernel density estimator

$$(3) \quad \hat{p}_h(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{c_d h^d} K\left(\frac{x - X_i}{h}\right) \quad \forall x \in \mathbb{R}^d,$$

where  $c_d \equiv \int_{\mathbb{R}^d} K(x) d\mu(x)$ . For simplicity, we assume that the kernel  $K : \mathbb{R}^d \mapsto \mathbb{R}_+$  is a symmetric, bounded, smooth function supported on the Euclidean unit ball. These assumptions can be easily relaxed to include, for instance, the case of regular kernels as defined in Devroye, Györfi and Lugosi [(1997), Chapter 10]. In particular, while the compactness of the support of  $K$  simplifies our analysis, it is not essential and could be replaced by assuming fast decaying tails. Further conditions on the kernel  $K$  are discussed in Section 3.1.

Let  $p_h : \mathbb{R}^d \mapsto \mathbb{R}$  be the measurable function given by

$$(4) \quad p_h(x) = \int_S K_h(x - y) dP(y) = \mathbb{E}(\hat{p}_h(x)),$$

where  $K_h(x) \equiv \frac{1}{c_d h^d} K\left(\frac{\|x\|}{h}\right)$ . Also, let  $K_h \mu$  be the probability measure given by  $K_h \mu(A) = \int_A K_h(x) d\mu(x)$ , for any Borel set  $A \subseteq \mathbb{R}^d$ . Then,  $p_h$  is the Lebesgue density of the probability measure  $P_h$  obtained by convolving  $P$  with  $K_h \mu$ . More precisely, for each measurable set  $A$ ,

$$P_h(A) = \int_A \int_S K_h(x - y) dP(y) d\mu(x) = \int_A p_h(x) d\mu(x).$$

Borrowing some terminology from analysis, where the kernel  $K$  is referred to as a mollifier, we call the measure  $P_h$  and the density  $p_h$  as the mollified measure and mollified density, respectively. For each  $h$ , the mollification of  $P$  by  $K$  yields that:

1. the mollified measure  $P_h$  has full-dimensional support  $S \oplus B(0, h)$  and is absolutely continuous with respect to  $\mu$ ; here, for two set  $A$  and  $B$  in  $\mathbb{R}^d$ ,  $A \oplus B \equiv \{x + y : x \in A, y \in B\}$  denotes its Minkowski sum;
2. the mollified density  $p_h$  is of class  $C^\alpha$  whenever  $K$  is of class  $C^\alpha$ , with  $\alpha \in \mathbb{N}_+ \cup \{\infty\}$ . (A real valued function is of class  $C^\alpha$  if its partial derivatives up to order  $\alpha$  exist and are continuous.)

(As a referee pointed out to us, the properties of mollified measures are related to the classical theory of distributions.) Mollifying  $P$  makes it better behaved. At the same time,  $P_h$  and  $p_h$  can be seen as approximations of the original measure  $P$  and the geometric density  $p$ , respectively, in a sense made precise by the following result.

LEMMA 1. *As  $h \rightarrow 0$ ,  $P_h$  converges weakly to  $P$  and  $\lim_{h \rightarrow 0} p_h(x) = p(x)$ , almost everywhere  $P$ .*

To estimate the  $\lambda$ -clusters of  $p$ , we use the connected components of  $\widehat{L}$ , that is, the  $\lambda$ -clusters of  $\widehat{p}_h$ . That is, we estimate  $L$  with

$$(5) \quad \widehat{L} \equiv \widehat{L}_h(\lambda) = \{x : \widehat{p}_h(x) \geq \lambda\}.$$

In practice, finding the estimated clusters is computationally difficult. Indeed, to verify that two points  $x_1$  and  $x_2$  are in the same cluster, we need to find at least one path  $\gamma \subset \mathbb{R}^d$  connecting them such that  $\widehat{p}_h(x) \geq \lambda$  for each  $x \in \gamma$ . Conversely, when  $x_1$  and  $x_2$  do not belong to the same cluster, this property has to be shown to fail for every possible path between them. We discuss an algorithm for approximating the clusters in Section 5. Until then, we ignore the computational problems and assume that the  $\lambda$ -clusters of  $\widehat{p}_h$  can be computed exactly.

2.2. *Risk.* We consider two different risk functions.

- The *level set risk* is defined to be  $R^L(p, \widehat{p}_h) = \mathbb{E}(\rho(p, \widehat{p}_h, P))$ , where

$$(6) \quad \rho(r, q, P) = \int_{\{x : r(x) \geq \lambda\} \Delta \{x : q(x) \geq \lambda\}} dP(x),$$

and  $A \Delta B = (A \cap B^c) \cup (A^c \cap B)$  is the symmetric set difference.

- Define the *excess mass functional* as

$$(7) \quad \mathcal{E}(A) = P(A) - \lambda \mu(A)$$

for any measurable set  $A \subset \mathbb{R}^d$ . This functional is maximized by the true level set  $L$ ; see Mueller and Sawitzki (1991) and Polonik (1995). We can use the

excess mass functional as a risk function except, of course, that we maximize it rather than minimize it. Given an estimate  $\widehat{L}$  of  $L$  based on  $\widehat{p}_h$ , we will then be interested in making the *excess mass risk*

$$(8) \quad R^M(p, \widehat{p}_h) = \mathcal{E}(L) - \mathbb{E}(\mathcal{E}(\widehat{L}))$$

as small as possible. Furthermore, if  $P$  has full-dimensional support, simple algebra reveals that maximizing  $\mathcal{E}(A)$  is equivalent to minimizing,

$$\int_{A \Delta L} |p - \lambda| d\mu,$$

which is the loss function used by Willett and Nowak (2007). In this case, the minimizer  $L$  is unique. More generally, if  $P = P_0 + P_1$  where  $P_0$  is the part of  $P$  that is absolutely continuous with respect to the Lebesgue measure, then

$$(9) \quad \mathcal{E}(L) - \mathcal{E}(A) = \int_{A \Delta L} |p_0 - \lambda| d\mu + P_1(L) - P_1(A),$$

where  $p_0 = \frac{dP_0}{d\mu}$ . It is clear that  $L$  is no longer the unique minimizer of the excess mass functional.

2.3. *Assumptions.* Throughout our analysis, we assume the following conditions.

(C1) There exist positive constants  $\gamma$ ,  $C_1$  and  $\bar{\varepsilon}$  such that

$$\mathbb{P}(|p(X) - \lambda| < \varepsilon) \leq C_1 \varepsilon^\gamma \quad \forall \varepsilon \in [0, \bar{\varepsilon}).$$

(C2) There exist a positive constant  $\bar{h}$ , and a permutation  $\sigma$  of  $\{1, \dots, k\}$  such that, for all  $h \in (0, \bar{h})$  and all  $\lambda' \in (\lambda - \bar{\varepsilon}, \lambda + \bar{\varepsilon})$ ,

$$L_h(\lambda') = \bigcup_{j=1}^k C_j^h(\lambda'),$$

where:

(a)  $C_i^h(\lambda') \cap C_j^h(\lambda') = \emptyset$  for  $1 \leq i < j \leq k$ ;

(b)  $C_j(\lambda') \subseteq C_{\sigma(j)}^h(\lambda')$ , for all  $1 \leq j \leq k$ .

(C3) There exist a positive constant  $C_2$  such that, for all  $h \in (0, \bar{h})$  and  $\lambda' \in (\lambda - \bar{\varepsilon}, \lambda]$ ,

$$L(\lambda') = \bigcup_{j=1}^k C_j(\lambda'),$$

where

$$\mu(\partial C_j(\lambda') \oplus B(0, h)) \leq C_2 h^{(d-d_i) \vee 1},$$

and  $d_i$  is the dimension of the component  $S_i$  of the support of  $P$  such that  $C_j(\lambda') \subseteq S_i$ .

2.4. *Remarks on the assumptions.* Conditions of the form (C1) or of other equivalent forms, are also known as low noise condition or margin conditions in the classification literature. They have appeared in many places, such as Tsybakov (1997), Mammen and Tsybakov (1999), Baïllo, Cuesta-Albertos and Cuevas (2001), Tsybakov (2004), Steinwart, Hush and Scovel (2005), Cuevas, González-Manteiga and Rodríguez-Casal (2006), Cadre (2006), Audibert and Tsybakov (2007), Castro and Nowak (2008) and Singh, Scott and Nowak (2009).

This condition, first introduced in Polonik (1995), provides a way to relate the stochastic fluctuations of  $\widehat{p}_h$  around its mean  $p_h$  to the clustering risk. Indeed, the larger  $\gamma$ , the smaller the effects of these fluctuations, and the easier it is to obtain good clusters from noisy estimates of  $p_h$ , for any  $h < \bar{h}$ .

Conditions (C2) simply require that the level set of the mollified density include the true clusters. The additional fringe  $L_h - L$  can be viewed as a form of clustering bias. Though mild and reasonable, these assumptions are particularly important, as they imply that the estimated density  $\widehat{p}_h$  can be used quite effectively for clustering purposes, for a range of bandwidth values. This is shown in the next simple result. Let  $N(\lambda)$ ,  $N_h(\lambda)$  and  $\widehat{N}_h(\lambda)$  denote the number of  $\lambda$ -clusters for  $p$ ,  $p_h$  and  $\widehat{p}_h$ , respectively. Notice that we do not require  $p$  to satisfy any smoothness properties. See Section 3.3 for the case case of smooth densities.

LEMMA 2. *Under conditions (C2) and for all  $\varepsilon \in (0, \bar{\varepsilon})$  and  $h \in (0, \bar{h})$ , on the event  $\mathcal{E}_{h,\varepsilon} = \{\|\widehat{p}_h - p_h\|_\infty < \varepsilon\}$ ,*

$$N_h(\lambda) = \widehat{N}_h(\lambda) = k.$$

Condition (C3) is used to obtain establish rates of convergence for the level set risk and the excess mass risk. It provides a way of quantifying the clustering bias due to the use of the mollified density  $p_h$  as a function of the bandwidth  $h$ , locally in a neighborhood of  $\lambda$ . In fact, if condition (C2) holds, then the clustering bias is due to the sets  $L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)$ , for  $h \in (0, \bar{h})$  and  $\varepsilon \in [0, \bar{\varepsilon})$ .

LEMMA 3. *Under conditions (C2) and (C3), for all  $h \in (0, \bar{h})$  and  $\varepsilon \in [0, \bar{\varepsilon})$  such that  $\lambda - \varepsilon \geq 0$ ,*

$$(10) \quad \mu(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \leq C_2 h^\theta,$$

where

$$\theta = \begin{cases} d - \max_i d_i + 1, & \text{if } \max_i d_i > 0, \\ d, & \text{otherwise,} \end{cases}$$

and, for some positive constant  $C_3$ ,

$$(11) \quad P(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \leq C_3 h^\xi,$$

where  $\xi$  is either  $\infty$  or 1; in particular,  $\xi = 1$  only if  $\max_i d_i = d$ .

Condition (C3) is rather mild and depends only on dimension of the support of  $P$ . Indeed, it follows from the rectifiability property (see the [Appendix](#) for details) that if,  $S_i$  is a component of the support of  $P$  of dimension  $d_i < d$ , then  $S_i$  has box-counting dimension  $d_i$  [see, e.g., [Ambrosio, Fusco and Pallara \(2000\)](#), Theorem 2.104]. This implies that (C3) is satisfied for all  $h$  small enough [see also [Falconer \(2003\)](#)]. For clusters  $C_j$  belonging to full-dimensional components of the support of  $P$ , (C3) follows if the sets  $\partial C_j(\lambda')$  have box-counting dimension  $d - 1$  for all  $\lambda' \in (\lambda - \bar{\varepsilon}, \lambda]$  and if  $\bar{h}$  is small enough. In fact, under these additional assumptions, it is possible to show that the bounds in Lemma 3 are sharp in the sense that, for all  $\lambda' \in (\lambda - \bar{\varepsilon}, \lambda]$  and  $h \in (0, \bar{h})$ ,  $\mu(L_h(\lambda') - L(\lambda')) = \Omega(h^\theta)$ . In addition, provided that  $\bar{h}$  is smaller than the minimal inter-cluster distance

$$\min_{i \neq j} \inf_{x \in C_j, y \in C_i} \|x - y\|,$$

we also obtain that  $P(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) = \Omega(h^\xi)$ , where  $\xi$  can only be 1 or  $\infty$ .

Finally, we point out that the value of  $\bar{h}$  depends on the curvature of the components  $\partial L(\lambda - \varepsilon)$  for all  $\varepsilon \in [0, \bar{\varepsilon})$ , and on the minimal inter-cluster distance. The smaller the condition numbers [see, e.g., [Niyogi, Smale and Weinberger \(2008\)](#)] of these components, and the larger the inter-cluster distance, the larger  $\bar{h}$ .

Although the rates are not affected by the constants, in practice, they can have a significant effect on the results, since they may very well depend on  $d$ . This is especially true of  $C_1$ , as illustrated in [Example 7](#) below.

*2.5. A refined analysis of condition (C1).* We conclude this section with some comments on the parameter  $\gamma$  appearing in condition (C1), whose value affects in a crucial way the consistency rates, with faster rates arising from larger values of  $\gamma$ . If  $S$  has dimension smaller than  $d$ , then, clearly,  $\gamma = \infty$ , thus throughout this subsection we assume that  $P$  is a probability measure on  $\mathbb{R}^d$  having Lebesgue density  $p$ .

First, a fairly general sufficient condition for assumption (C1) to hold with  $\gamma = 1$  at  $\lambda$  can be easily obtained using probabilistic arguments as follows. Let  $G$  denote the distribution of the random variable  $Y = p(X)$  and suppose  $G$  has a Lebesgue density  $g$  which is bounded away from 0 and infinity on  $(\lambda - \bar{\varepsilon}, \lambda + \bar{\varepsilon})$ . Then, by the mean value theorem, for any nonnegative  $\varepsilon < \bar{\varepsilon}$ ,

$$\mathbb{P}(\lambda - \varepsilon \leq p(X) \leq \lambda + \varepsilon) = G(\{y : y \in (\lambda + \varepsilon, \lambda - \varepsilon)\}) = \varepsilon g(\lambda + \eta)$$

for some  $\eta \in (-\varepsilon, \varepsilon)$ . Thus, (C1) holds with  $\gamma = 1$  at  $\lambda$ . See also [Example 7](#) below. A more refined result based on analytic conditions is given next. Below  $\mathcal{H}^{d-1}$  denotes the  $(d - 1)$ -dimensional Hausdorff measure in  $\mathbb{R}^d$ . See the [Appendix](#) for the definition of Hausdorff measure.



LEMMA 4. *Suppose that  $P$  is a probability measure on  $\mathbb{R}^d$  having Lipschitz density  $p$ . Assume that, almost everywhere  $\mu$ ,  $\|\nabla p(x)\| > 0$  and that  $\mathcal{H}^{d-1}(\{x : p(x) = \lambda\}) < \infty$  for any  $\lambda \in (0, \|p\|_\infty)$ . Then (C1) holds with  $\gamma = 1$  for each  $\lambda \in (0, \|p\|_\infty)$  except for a set of Lebesgue measure 0.*

A further point of interest is to characterize the set of  $\lambda$  values for which condition (C1) holds with  $\gamma \neq 1$ . Clearly, if  $p$  has a jump discontinuity, then (C1) holds with  $\gamma = \infty$ , for all values of  $\lambda$  in some interval. On the other hand, due to the previous result, if  $\|\nabla p\|$  is bounded away from 0 and  $\infty$  in a neighborhood of  $p^{-1}(\lambda)$ , then  $\gamma = 1$ . Thus, one could expect a value of  $\gamma$  different than 1 when  $\nabla p$  does not exist or when  $\|\nabla p\|$  is infinity or vanishes in  $p^{-1}(\lambda)$ . See the example on page 7 in Rigollet and Vert (2006), where (C1) holds with  $\gamma < 1$  if  $q > d$  and  $\gamma > 1$  if  $q < d$ , the former case corresponding to  $\|\nabla p(x_0)\| = 0$  and the latter to  $\lim_{x \rightarrow x_0} \|\nabla p(x)\| = \infty$ . However, this would seem to indicate that, if  $p$  is sufficiently regular, the values of  $\lambda$  for which  $\gamma \neq 1$  form a negligible set of  $\mathbb{R}$ . Lemma 4 above already shows that this set has Lebesgue measure zero if  $p$  is Lipschitz with nonvanishing gradient. Under stronger assumptions, it can be verified that this set is in fact finite.

COROLLARY 5. *Under the assumption of Lemma 4, if  $p$  is of class  $\mathcal{C}^1$  and has compact support, then the set of  $\lambda$  such that (C1) holds with  $\gamma \neq 1$  is finite.*

EXAMPLE 6. *Sharp clusters and lower-dimensional clusters. Suppose that  $p = \frac{dP}{d\mu} = \sum_{i=1}^m \pi_j p_j$  where  $p_i$  is a density with support on a compact, connected set  $S_i$ ,  $\sum_i \pi_i = 1$  and  $\min_i \pi_i > 0$ . Moreover, suppose that*

$$\min_{i \neq j} \inf_{x \in C_i, y \in C_j} \|x - y\| > 0,$$

where  $d(A, B) = \inf_{x \in A, y \in B} \|x - y\|$ . Finally, suppose that

$$\min_j \inf_{x \in C_j} \pi_j p(x) \geq \lambda.$$

We denote clusters of this type as sharp clusters. See Singh, Nowak and Zhu (2008), for example. It is easy to see that (C1) and (11) hold with  $\gamma = \xi = \infty$ . A more general example in which one of the mixture component is supported on a lower dimensional set is shown in Figure 1. Here, the true distribution is  $P = (1/3) \text{Unif}(-5.5, -4.5) + (1/3) \text{Unif}(4.5, 5.5) + (1/3)\delta_0$ . The geometric density and the mollified density based on  $h = 0.04$  are shown in the top plot. The point mass at 0 is indicated with a vertical bar. The bottom plot shows the true clusters and the mollified clusters based on  $p_h$  with  $\lambda = 0.04$ . The clusters based on  $p_h$  contain the true clusters and the difference between them is a set of zero probability.

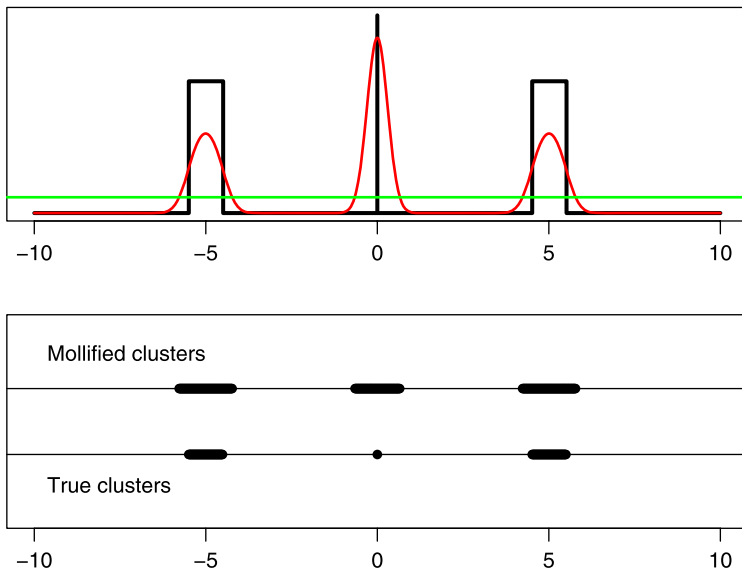


FIG. 1. Sharp clusters. Top: the density of  $P = (1/3) \text{Unif}(-5.5, -4.5) + (1/3) \text{Unif}(4.5, 5.5) + (1/3)\delta_0$  and the mollified density  $p_h$  for  $h = 0.04$ . The point mass at 0 is indicated with a vertical bar. Bottom: the true clusters and the mollified clusters of  $p_h$  with  $\lambda = 0.04$ .

EXAMPLE 7 (Normal distributions). Suppose that  $X \sim N_d(0, \Sigma)$ , with  $\Sigma$  positive definite. Set  $\sigma = |\Sigma|^{1/2}$ . Then (C1) holds for any  $0 \leq \lambda \leq (\sigma(\sqrt{2\pi})^d)^{-1}$  with  $\gamma = 1$  and  $C_1 = C_d 2\sigma(\sqrt{2\pi})^d$ , where the constant  $C_d$  depends on  $d$  (and, of course,  $\lambda$ ). We prove the claim only for  $\lambda = \alpha(\sigma(\sqrt{2\pi})^d)^{-1}$ , where  $\alpha \in (0, 1)$ . Cases in which  $\alpha = 1$  or  $\alpha = 0$  can be dealt with similarly. Let  $W \sim \chi_d^2$  and notice that  $X^\top \Sigma^{-1} X \stackrel{d}{=} W$ . For all  $\varepsilon > 0$  smaller than

$$(12) \quad \min \left\{ \frac{\alpha}{\sigma(\sqrt{2\pi})^d}, \frac{(1-\alpha)}{\sigma(\sqrt{2\pi})^d} \right\},$$

simple algebra yields

$$\begin{aligned} & P(|\phi_\sigma(X) - \lambda| < \varepsilon) \\ &= \mathbb{P} \left( 2 \log \frac{1}{\alpha - \varepsilon \sigma(\sqrt{2\pi})^d} \leq W \leq 2 \log \frac{1}{\alpha + \varepsilon \sigma(\sqrt{2\pi})^d} \right) \\ &= 2 \left( \log \frac{1}{\alpha - \varepsilon(\sigma\sqrt{2\pi})^d} - \log \frac{1}{\alpha + \eta\sigma(\sqrt{2\pi})^d} \right) p_d \left( \log \frac{1}{\alpha + \eta\sigma(\sqrt{2\pi})^d} \right) \end{aligned}$$

for some  $\eta \in (-\varepsilon, \varepsilon)$  where  $p_d$  denotes the density of a  $\chi_d^2$  distribution and the second equality holds in virtue of the mean value theorem. By a first order Taylor expansion, for  $\varepsilon \downarrow 0$ , the first term on the right-hand side of the previous display

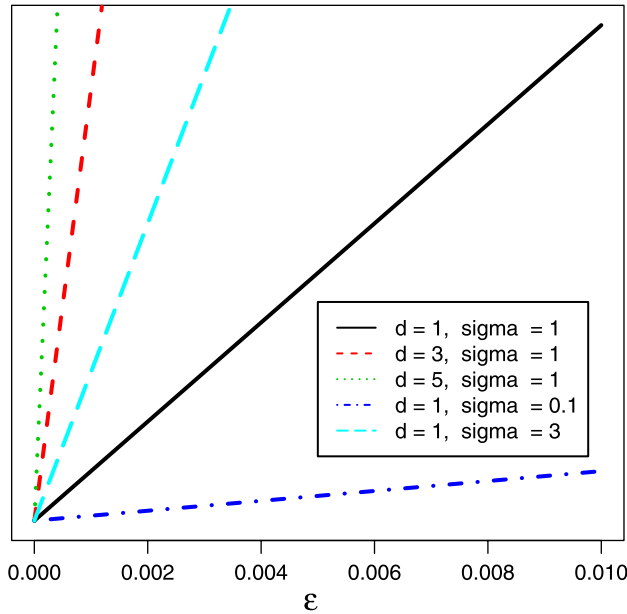


FIG. 2. Noise exponent for Gaussians. Each curve shows  $\mathbb{P}(|p(X) - \lambda| < \varepsilon)$  versus  $\varepsilon$  for  $\alpha = 1/2$ . The plots are nearly linear since  $\gamma = 1$  in this case.

can be written as

$$2\varepsilon\sigma(\sqrt{2\pi})^d \left( \frac{1}{\alpha - \varepsilon\sigma(\sqrt{2\pi})^d} + \frac{1}{\alpha + \varepsilon\sigma(\sqrt{2\pi})^d} \right) + o(\varepsilon^2).$$

Since  $(\frac{1}{\alpha - \varepsilon\sigma(\sqrt{2\pi})^d} + \frac{1}{\alpha + \varepsilon\sigma(\sqrt{2\pi})^d}) p_d(\log \frac{1}{\alpha + \eta\sigma(\sqrt{2\pi})^d}) \asymp 1$  for any  $\varepsilon \geq 0$  bounded by (12), the claim is proved. See Figure 2.

**3. Rates of convergence.** In this section, we study the rates of convergence in the two distances using deterministic bandwidths. We defer the discussion of random (data driven) bandwidths until Section 4.

3.1. *Preliminaries.* Before establishing consistency rates for the different risk measures described above, we discuss some necessary preliminaries.

In our analysis, we require the event

$$(13) \quad \mathcal{E}_{h,\varepsilon} \equiv \{\|\hat{p}_h - p_h\|_\infty \leq \varepsilon\}, \quad \varepsilon \in (0, \bar{\varepsilon}), h \in (0, \bar{h}),$$

to hold with high probability, for all  $n$  large enough. In fact, some control over  $\mathcal{E}_{h,\varepsilon}$  provides a means of bounding the clustering risks, as shown in the following result.

LEMMA 8. *Let  $\varepsilon \in (0, \bar{\varepsilon})$  and  $h \in (0, \bar{h})$  be such that the conditions (C1) and (C2) are satisfied. Then, on the event  $\mathcal{E}_{h,\varepsilon}$ ,*

$$L(\lambda + \varepsilon) \subseteq \widehat{L}_h(\lambda) \subseteq L(\lambda + \varepsilon) \cup A \cup B,$$

where

$$A = L(\lambda - \varepsilon) - L(\lambda + \varepsilon)$$

and

$$B = L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon).$$

Therefore, on  $\mathcal{E}_{h,\varepsilon}$ , under the additional condition (C3),

$$(14) \quad P(\widehat{L}_h(\lambda) \Delta L(\lambda)) \leq C_1 \varepsilon^\nu + C_2 h^\xi.$$

In order to bound  $\mathbb{P}(\mathcal{E}_{h,\varepsilon}^c)$ , we study the properties of the kernel estimator  $\widehat{p}_h$ . We will impose the following condition on the kernel  $K$ .

(VC) The class of functions

$$\mathcal{F} = \left\{ K\left(\frac{x - \cdot}{h}\right), x \in \mathbb{R}^d, h > 0 \right\}$$

satisfies, for some positive number  $A$  and  $v$

$$(15) \quad \sup_P N(\mathcal{F}_h, L_2(P), \varepsilon \|F\|_{L_2(P)}) \leq \left(\frac{A}{\varepsilon}\right)^v,$$

where  $N(T, d, \varepsilon)$  denotes the  $\varepsilon$ -covering number of the metric space  $(T, d)$ ,  $F$  is the envelope function of  $\mathcal{F}$  and the supremum is taken over the set of all probability measures on  $\mathbb{R}^d$ . The quantities  $A$  and  $v$  are called the VC characteristics of  $\mathcal{F}$ .

Assumption (VC) appears in [Giné and Guillou \(2002\)](#), [Einmahl and Mason \(2005\)](#), and [Giné and Koltchinskii \(2006\)](#). It holds for a large class of kernels, including, for example, any compact supported polynomial kernel and the Gaussian kernel. See [Nolan and Pollard \(1987\)](#) and [van der Vaart and Wellner \(1996\)](#) for sufficient conditions for (VC).

Using condition (VC), we can establish the following finite sample bound for  $\mathbb{P}(\|\widehat{p}_h - p_h\|_\infty > \varepsilon)$ , which is obtained as a direct application of results in [Giné and Guillou \(2002\)](#).

PROPOSITION 9 (Gine and Guillon). *Assume that the kernel satisfies the property (VC) and that*

$$(16) \quad \sup_{t \in \mathbb{R}^d} \sup_{h > 0} \int_{\mathbb{R}^d} K_h^2(t - x) dP(x) < D < \infty.$$

1. Let  $h$  be fixed. Then, there exist constants  $L > 0$  and  $C > 0$ , which depend only on the VC characteristics of  $K$ , such that, for any  $c_1 \geq C$  and  $0 < \varepsilon \leq \frac{c_1 D}{\|K\|_\infty}$ , there exists an  $n_0 > 0$ , which depends on  $\varepsilon, D, \|K\|_\infty$  and the VC characteristics of  $K$ , such that, for all  $n \geq n_0$ ,

$$(17) \quad \mathbb{P}\left\{ \sup_{x \in \mathbb{R}^d} |\widehat{p}_h(x) - p_h(x)| > 2\varepsilon \right\} \leq L \exp\left\{ -\frac{1}{L} \frac{\log(1 + c_1/(4L))}{c_1} \frac{nh^d \varepsilon^2}{D} \right\}.$$

2. Let  $h_n \rightarrow 0$  as  $n \rightarrow \infty$  in such a way that  $\frac{nh_n^d}{|\log h_n^d|} \rightarrow \infty$ . If  $\{\varepsilon_n\}$  is a sequence such that

$$(18) \quad \varepsilon_n = \Omega\left(\sqrt{\frac{\log r_n}{nh_n^d}}\right),$$

where  $r_n = \Omega(h_n^{-d/2})$ , then, for all  $n$  large enough, (17) holds with  $h$  and  $\varepsilon$  replaced by  $h_n$  and  $\varepsilon_n$ , respectively. In particular, the term on the right-hand side of (17) vanishes at the rate  $O(r_n^{-1})$ .

The above theorem imposes minimal assumptions on the kernel  $K$  and, more importantly, on the probability distribution  $P$ , whose density is not required to be bounded or smooth, and, in fact, may not even exist. Condition (16) is automatically satisfied by bounded kernels. Finally, we remark that, for fixed  $h$ , setting  $\varepsilon_n = \sqrt{\frac{2 \log n}{h^d n C_K}}$  for an appropriate constant  $C_K$  (depending on  $K$ ), an application of the Borel–Cantelli lemma yields that, as  $n \rightarrow \infty$ ,  $\|p_h - \widehat{p}_h\|_\infty = O(\sqrt{\frac{\log n}{n}})$  almost everywhere  $P$ .

**3.2. Rates of convergence.** We now derive the converge rates for the clustering risks defined in Section 2.2. Below, we will write  $C_K$  for a constant whose value depends only on the VC characteristic of the kernel  $K$  and on the constant  $D$  appearing in (16).

We recall that Lemma 3 provides a way of controlling the clustering bias due to the sets  $L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)$ , uniformly over  $\varepsilon < \bar{\varepsilon}$  and  $h < \bar{h}$ . In fact, the parameters  $\theta \in \{1, \dots, d\}$  and  $\xi \in \{1, \infty\}$  will determine the rates of consistency for the excess mass and the level set risk, respectively. Specifically, higher values of the parameter  $\theta$  which correspond to supports of lower dimension yield faster convergence rates for the excess mass risk. As for the level set risks, the case  $\xi = \infty$  is the most favorable, since it implies that the clustering bias has no effect on the estimation of level sets and dimension independent rates are possible. In particular, if  $C_j$  has dimension smaller than  $d$ , then  $P(C_{\sigma(j)}^h - C_j) = 0$ , so that  $\xi = \infty$ . More generally,  $\xi = \infty$  occurs when  $L = S$ . Overall our results yield that, as expected, better rates for the clustering risk are obtained for distributions supported on lower-dimensional sets.

**THEOREM 10 (Level set risk).** *Suppose that (C1), (C2), (C3) and (VC) hold. Then there exists a constant  $C_L$  such that, for any  $h \in (0, \bar{h})$  and  $\varepsilon \in (0, \bar{\varepsilon})$ ,*

$$(19) \quad R^L(p, \hat{p}_h) \leq C_L(\varepsilon^\gamma + h^\xi + e^{-C_K n h^d \varepsilon^2}).$$

*In particular, setting*

$$h_n = \left(\frac{\log n}{n}\right)^{\gamma/(2\xi+d\gamma)} \quad \text{and} \quad \varepsilon_n = \sqrt{\frac{\log n}{C_K n h_n^d}}$$

*we obtain*

$$(20) \quad R^L(p, \hat{p}_{h_n}) = O\left(\max\left\{\left(\frac{\log n}{n}\right)^{\gamma\xi/(2\xi+d\gamma)}, \frac{1}{n}\right\}\right).$$

If  $\gamma = \infty$ , then either  $S - L$  is empty or has zero Lebesgue measure, or  $S - L$  is a full dimensional set of positive Lebesgue measure. The former cases, which correspond to  $P$  having a lower-dimensional support or to sharp clusters (see Example 6), implies that  $R^L = O(\frac{1}{n})$ . Thus, we have dimension independent rates for sharp clusters. In the latter case,  $\xi = 1$ , so that  $R^L$  is of order  $O((\frac{\log n}{n})^{1/d})$ . When  $\gamma < \infty$ , then  $\xi = 1$  and the risk is of order  $O((\frac{\log n}{n})^{\gamma/(2+d\gamma)})$ .

In practice, there are examples in between the sharp and nonsharp cases for probability distributions with full-dimensional support. For example, if there is a very small amount of mass just outside the cluster, then, technically,  $\xi = 1$  and the rate will be slow for large  $d$ . However, if this mass is very small then we expect for finite samples that the behavior of the risk will be close to the behavior observed in the sharp case. We could capture this idea mathematically by allowing  $P$  to change with  $n$  and then allowing  $\xi_n$  to vary with  $n$  and take values between 1 and  $\infty$ . However, we shall not pursue the details here.

As an interesting corollary to Theorem 10, we can show that the expected proportion of sample points that are incorrectly assigned as clusters or noise vanishes at the same rate.

**COROLLARY 11.** *Let  $\hat{f}_h = \frac{|\hat{J}_h|}{n}$ , where*

$$\hat{I}_h = \{i : \text{sign}(\hat{p}_h(X_i) - \lambda) \neq \text{sign}(p(X_i) - \lambda)\}.$$

*Then,  $\mathbb{E}(\hat{f}_h) \leq C_L(\varepsilon^\gamma + h^\xi + e^{-C_K n h^d \varepsilon^2})$ .*

We now turn to the excess mass risk.

**THEOREM 12 (Excess mass).** *Suppose that (C1), (C2), (C3) and (VC) hold. Then, there exists a constant  $C_M$ , independent of  $\varepsilon$  and  $h$ , such that, for any  $h \in (0, \bar{h})$  and  $\varepsilon \in (0, \bar{\varepsilon})$  with  $\varepsilon < \lambda$ ,*

$$R^M(p, \hat{p}_h) \leq C_M(\varepsilon^{\gamma+1} + h^\theta + e^{-n C_K \varepsilon^2 h^d}).$$

Thus, setting

$$h_n = \left(\frac{\log n}{n}\right)^{(\gamma+1)/(2\theta+d(\gamma+1))} \quad \text{and} \quad \varepsilon_n = \sqrt{\frac{\log n}{C_K n h_n^d}},$$

we obtain

$$(21) \quad R^M(p, \hat{p}_h) = O\left(\left(\frac{\log n}{n}\right)^{\theta(\gamma+1)/(2\theta+d(\gamma+1))}\right).$$

When  $\gamma = \infty$  the excess mass risk  $R^M$  is of order  $O\left(\frac{\log n}{n}\right)^{\theta/d}$ . Thus, the higher  $\theta$ , that is, the smaller the dimension of the support of  $P$ , the faster the rate of convergence. In particular, if  $P$  is supported over a finite set of points the risk vanishes at the dimension independent rate  $O\left(\frac{\log n}{n}\right)$ . When  $\gamma < \infty$ , then  $\theta = 1$  and the risk is of order  $O\left(\left(\frac{\log n}{n}\right)^{(\gamma+1)/(2+d(\gamma+1))}\right)$ .

3.3. *Some special cases.* Here, we discuss some interesting special cases.

*Fast rates for biased clusters.* In some cases, we might be content with estimating the level set  $L_h(\lambda)$ , which is a biased version of  $L(\lambda)$ . That is, the fringe  $L_h(\lambda) - L(\lambda)$  may not be of great practical concern and, in fact, it may contain a very small amount of mass. Indeed, we believe this is why clustering is often so successful in high-dimensional problems. Exact estimation of the level sets is not necessary in many practical problems. In fact, by Lemma 2, conditions (C2) guarantees that  $\hat{L}$  will include  $L$  with high probability. Thus, for clustering purposes, one may consider some modifications of our risk functions. First, suppose we only require that the estimated clusters cover the true clusters. That is, we say there is not error as long as  $C_j \subset \hat{C}_j$ . This suggests the following modification of our risk functions:

- $\tilde{R}^L(p, \hat{p}_h) = \int_{\{x: p(x) \geq \lambda\} \cap \{x: \hat{p}_h(x) < \lambda\}} dP(x),$
- $\tilde{R}^M(p, \hat{p}_h) = \mathcal{E}(L) - \mathbb{E}(\hat{L}_h \cap L).$

Then we have the following result, which gives faster, dimension independent rates. The proof is similar to the proofs of the previous results and is omitted.

**THEOREM 13.** *Let  $h \in (0, \bar{h})$  be fixed. Under (C1), (C2) and (VC), then*

$$\tilde{R}^L(p, \hat{p}_h) = O\left(\max\left\{\left(\frac{\log n}{n}\right)^{\gamma/2}, \frac{1}{n}\right\}\right)$$

and

$$\tilde{R}^M(p, \hat{p}_h) = O\left(\left(\frac{\log n}{n}\right)^{(1+\gamma)/2}\right).$$

Alternatively, one may be only interested in estimating the clusters of the mollified density  $p_h$ , for any fixed  $h \in (0, \bar{h})$ . Then, provided that  $p_h$  is sufficiently smooth (which is guaranteed by choosing a smooth kernel) and has finite positive gradient for each point in the set  $\partial L_h(\lambda)$ , the results in Section 2.5 show that, for all  $\varepsilon$  small enough,

$$\mu(\{x : |p_h(x) - \lambda| < \varepsilon\}) \leq \varepsilon.$$

Thus, under assumptions (C2) and (VC), similar arguments to the ones used in the proofs of Theorems 10 and 12 imply that

$$R^L(p_h, \hat{p}_h) = \int_{\{x: p_h(x) \geq \lambda\} \Delta \{x: \hat{p}_h(x) \geq \lambda\}} dP(x) = O\left(\sqrt{\frac{\log n}{n}}\right)$$

and

$$R^M(p_h, \hat{p}_h) = \mathcal{E}(L_h) - \mathbb{E}(\mathcal{E}(\hat{L}_h)) = O\left(\frac{\log n}{n}\right).$$

In either case, we get dimension independent rates.

*The smooth full-dimensional case.* In the more specialized settings in which  $P$  has full-dimensional support and the Lebesgue density  $p$  is smooth, better results are possible. For example, using the same settings of Rigollet and Vert (2006), if  $p$  is  $\beta$ -times Hölder differentiable, then the bias conditions (C2) are superfluous, as

$$(22) \quad \|p_h - p\|_\infty \leq Ch^\beta$$

for some constant  $C$  which depends only on the kernel  $K$ . Choosing  $h$  such that  $Ch^\beta < \varepsilon$ , on the event  $\mathcal{E}_{h,\varepsilon}$ , the triangle inequality yields  $\|\hat{p}_h - p\|_\infty < 2\varepsilon$ . Thus, for each  $\varepsilon < \frac{\varepsilon}{2}$  and each  $h$  such that  $Ch^\beta < \varepsilon$ , on  $\mathcal{E}_{h,\varepsilon}$ , instead of (14), one obtains

$$P(\hat{L}_h(\lambda) \Delta L(\lambda)) \leq C_1 2^\gamma \varepsilon^\gamma.$$

Then, setting  $h_n = (\log n/n)^{1/(2\beta+d)}$  and  $\varepsilon_n = \Omega((\log n/n)^{\beta/(2\beta+d)})$ , we see that  $R^L(p, \hat{p}_h)$  is of order  $O((\log n/n)^{\gamma\beta/(2\beta+d)})$ , while  $R^M(p, \hat{p}_h)$  is of order  $O((\log n/n)^{(\gamma+1)\beta/(2\beta+d)})$ . These, are, up to an extra logarithmic factor, the minimax rates established by Rigollet and Vert (2006). In fact, under these smoothness assumptions, and since the bias can be uniformly controlled as in (22), then, by a combination of Fubini's theorem and of a peeling argument as in Audibert and Tsybakov (2007) and Rigollet and Vert (2006), the exponential term  $O(e^{-C_K n h^d \varepsilon^2})$  becomes redundant and rates without the logarithmic term are possible.

**4. Choosing the bandwidth.** In this section, we discuss two data-driven method for choosing the bandwidth that adapts to the unknown parameters  $\gamma$  and  $\theta$ . Before we explain the details, we point out that  $L_2$  cross-validation is not appropriate for this problem. In fact, we are allowing for the case where  $P$  may have atoms, in which case it is well known that cross-validation chooses  $h = 0$ .



4.1. *Excess mass.* We propose choosing  $h$  by splitting the data and maximizing an empirical estimate of the excess mass functional. Polonik (1995) used this approach to choose a level set from among a fixed class  $\mathcal{L}$  of level sets of finite VC dimension. Here, we are choosing a bandwidth, or, in other words, we are choosing a level set from a random class of level sets  $\mathcal{L} = \{ \{x : \hat{p}_h(x) \geq \lambda\} : h > 0 \}$  depending on the observed sample  $X$ . The steps are in Table 1.

To implement the method, we need to compute  $\mu(L_h)$ . In practice,  $\mu(L_h)$  can be approximated by

$$\frac{1}{M} \sum_{i=1}^M \frac{I(\hat{p}_h(U_i) \geq \lambda)}{g(U_i)},$$

where  $U_1, \dots, U_M$  is a sample from a convenient density  $g$ . In particular, one can choose  $g = \hat{p}_H$  for some large bandwidth  $H$ . Choosing  $M \approx n^2$  ensures that the extra error of this importance sampling estimator is  $O(1/n)$  which is negligible. We ignore this error in what follows.

Technically, the method only applies for  $\lambda > 0$ , at least in terms of the theory that we derive. In practice, it can be used for  $\lambda = 0$ . In this case,  $\hat{\mathcal{E}}(h)$  becomes 1 when  $h$  is large. We then take  $\hat{h}$  to be the smallest  $h$  for which  $\hat{\mathcal{E}}(h) = 1$ .

Below we use the notation  $\mathcal{E}_X(\cdot)$  instead of  $\mathcal{E}(\cdot)$  to indicate that the excess mass functional (7) is evaluated at a random set depending on the training set  $X$  and, therefore, is itself random. Accordingly, with some abuse of notation, for any  $h > 0$ , we will write  $\mathcal{E}_X(h) = \mathcal{E}(L_h)$ , with  $L_h$  the  $\lambda$ -level set of  $\hat{p}_h$ . Below  $\mathcal{H}$  is a countable dense subset of  $[0, \bar{h}]$ . The next result is closely related to Theorem 7.1 of Györfi et al. (2002).

**THEOREM 14.** *Let  $h_* = \arg \max_{h \in \mathcal{H}} \mathcal{E}_X(h)$ . For any  $\delta > 0$ ,*

$$(23) \quad \mathbb{E}(\mathcal{E}_X(h_*)) - \mathbb{E}(\mathcal{E}_X(\hat{h})) \leq d(\delta, \kappa) \frac{1 + \log 2}{n},$$

where the expectation is with respect to the joint distribution of the training and test set,  $d(\delta, \kappa) = \frac{2}{\kappa} \delta(1 + \delta)(16\gamma^2 + \delta(7 + 16\gamma^2))$ , with  $\kappa = 2 + \lambda\mu(S + B(0, \bar{h}))$  and  $\gamma^2 = \frac{7}{4}(e^{4/7} - 1)$ .

TABLE 1  
Selecting the bandwidth using the excess mass risk

- 
1. Split the data into two halves which we denote by  $X = (X_1, \dots, X_n)$  and  $Z = (Z_1, \dots, Z_n)$ .
  2. Let  $\mathcal{H}$  be a finite set of bandwidths. Using  $X$ , construct kernel density estimators  $\{\hat{p}_h : h \in \mathcal{H}\}$ .  
Let  $L_h = \{x : \hat{p}_h(x) \geq \lambda\}$ .
  3. Using  $Z$ , estimate the excess mass functional

$$\hat{\mathcal{E}}(h) = \frac{1}{n} \sum_{i=1}^n I(Z_i \in L_h) - \lambda\mu(L_h).$$

4. Let  $\hat{h}$  be the maximizer of  $\hat{\mathcal{E}}(h)$  and set  $\hat{L} = L_{\hat{h}}$ .
-

Now we construct a grid  $\mathcal{H}_n$  of size depending on  $n$  that is guaranteed to ensure that optimizing over  $\mathcal{H}_n$  implies we are adapting over  $\gamma$  and  $\theta$ .

**THEOREM 15.** *Suppose (C1) and (C2) hold. Let*

$$\delta_n(\theta) = \frac{a_n^{\theta/d}}{2A_n(\theta)},$$

where  $a_n = (\log n/n)$  and

$$A_n(\theta) = \frac{2|\log a_n| a_n^{\theta/(2\theta+d)} \theta^2}{(2\theta + d)^2}.$$

Let  $G_n(\theta) = \{\gamma_1(\theta), \dots, \gamma_{N(\theta)}(\theta)\}$  where  $\gamma_j(\theta) = (j - 1)\delta_n(\theta)$  and  $N(\theta)$  is the smallest integer less than or equal to  $\Upsilon_n(\theta)/\delta_n(\theta)$ ,

$$\Upsilon_n(\theta) = \frac{2\theta^2}{d^2 W_n} - \frac{2\theta}{d} - 1$$

and

$$W_n = \frac{\log 2}{\log n - \log \log n}.$$

Let

$$\mathcal{H}_n = \{h_n(\gamma, \theta) : \theta \in \{1, \dots, d\}, \gamma \in G_n(\theta)\},$$

where  $h_n(\gamma, \theta) = a_n^{(\gamma+1)/(2\theta+d(\gamma+1))}$ . Let  $\widehat{L}$  be obtained by minimizing  $\widehat{\mathcal{E}}(h)$  for  $h \in \mathcal{H}_n$ . Then

$$\mathcal{E}(L) - \mathbb{E}(\mathcal{E}(\widehat{L})) \leq O\left(\frac{\log n}{n}\right)^{\theta(\gamma+1)/(2\theta+d(\gamma+1))}.$$

The latter theorem shows that our cross-validation methods gives a completely data-driven method for choosing the bandwidth that preserves the rate. Notice, in particular, that adapting to the parameter  $\theta$  is equivalent to adapting to the unknown dimension of the support of  $P$ . This makes it possible to use our method in practical problems as long as the sample size is large. For small sample sizes, data splitting might lead to highly variable results in which case our bandwidth selection method might not work well. An alternative is to split the data many times and combines the estimates over multiple splits.

When  $\mu(L) = 0$ , we have that  $h_* = 0$ . The above theorems are still valid in this case. Thus, the case where  $P$  is atomic is included while it is ruled out for  $L_2$  cross-validation.

4.2. *Stability.* Another method for selecting the bandwidth is to choose the value for  $h$  that produces stable clusters, in a sense defined below. The use of stability has gained much popularity in clustering; see Ben-Hur, Elisseeff and Guyon (2002) and Lange et al. (2004), for example. In the context of  $k$ -means clustering and related methods, Ben-David, von Luxburg and Pall (2006) showed that minimizing instability leads to poor clustering. Here, we investigate the use of stability for density clustering.

Suppose, for simplicity, that the sample size is a multiple of 3. That is, the sample size is  $3n$  say. Now randomly split the data into three vectors of size  $n$ , denoted by  $X = (X_1, \dots, X_n)$ ,  $Y = (Y_1, \dots, Y_n)$  and  $Z = (Z_1, \dots, Z_n)$ . (In practice, we split the data into three approximately equal subsets.)

We define the *instability function* as the random function  $\Xi : [0, \infty) \mapsto [0, 1]$  given by

$$(24) \quad \Xi(h) \equiv \rho(\hat{p}_h, \hat{q}_h, \hat{P}_Z) = \int_{\{x : \hat{p}_h(x) \geq \lambda\} \Delta \{x : \hat{q}_h(x) \geq \lambda\}} d\hat{P}_Z(x),$$

where  $\hat{p}_h$  is constructed from  $X$ ,  $\hat{q}_h$  is constructed from  $Y$  and  $\hat{P}_Z$  is the empirical distribution based on  $Z$ .

Rather than studying stability in generality, we consider a special case involving the following extra conditions.

1. *Sharp clusters.* Assume that  $P = \sum_{j=1}^m \pi_j P_j$  where  $\sum_i \pi_j = 1$ , and  $P_j$  is uniform on the compact set  $S_j$  of full dimension  $d$ . Thus,  $p(z) = \sum_j \Delta_j I(z \in S_j)$  where  $\Delta_j = \pi_j / \mu(S_j)$ . Let  $\underline{\Delta} = \min_j \Delta_j > 0$  and let  $\bar{\Delta} = \max_j \Delta_j$ .
2. *Spherical Kernel.* We use a spherical kernel so that

$$\hat{p}_h(z) = \frac{1}{nh^d} \sum_{i=1}^n \frac{I(\|z - X_i\| \leq h)}{v_d} = \frac{\hat{P}(B(z, h))}{h^d v_d},$$

where  $v_d = \pi^{d/2} / \Gamma(d/2 + 1)$  denotes the volume of the unit ball and  $\hat{P}$  is the empirical measure.

3. *The support of  $P$  is a standard set.* Letting  $S = \cup_{j=1}^m S_j$ , we assume that there exists a  $\delta \in (0, 1)$  such that

$$\mu(B(z, h) \cap L) \geq \delta \mu(B(z, h)) \quad \text{for all } z \in S \text{ and all } h < \text{diam}(S),$$

where  $\text{diam}(S) = \sup_{(x,y) \in S} \|x - y\|$  indicates the diameter of the set  $S$ . This property appears in a natural way in set estimation problems; see, for example, Cuevas and Fraiman (1997).

4. *Choice of  $\lambda$ .* We take  $\lambda = 0$ , so that  $L = S$ .

Under these settings, the graph  $\Xi(h)$  is typically unimodal with  $\Xi(0) = \Xi(\infty) = 0$ . Hence, it makes no sense to minimize  $\Xi$ . Instead, we will fix a constant  $\alpha \in (0, 1)$  and choose

$$(25) \quad \hat{h} = \inf \left\{ h : \sup_{t > h} \Xi(t) \leq \alpha \right\}.$$

**THEOREM 16.** *Let  $h_* = \text{diam}(L)$ . Under conditions 1–4:*

1.  $\Xi(0) = 0$  and  $\Xi(h) = 0$ , for all  $h \geq h_*$ ;
2.  $\sup_{0 < h < h_*} \mathbb{E}(\Xi(h)) \leq 1/2$ ;
3. as  $h \rightarrow 0$ ,  $\mathbb{E}(\Xi(h)) \asymp h^d$ ;
4. for each  $h \in (0, h_*)$ ,

$$D_3(h_* - h)^{d(n+1)} D_4^n \leq \mathbb{E}(\Xi(h)) \leq 2D_1(h_* - h)^{n+1} D_2^n,$$

where

$$D_1 = \frac{\pi^{d/2} h_*^{d-1}}{2^d \Gamma((d/2) + 1)}, \quad D_2 = \frac{\pi^{d/2} h_*^{d-1}}{\Gamma((d/2) + 1)},$$

$$D_3 = \frac{\delta \underline{\Delta} \pi^{d/2}}{\Gamma((d/2) + 1)}, \quad D_4 = \frac{\underline{\Delta} \delta \pi^{d/2}}{\Gamma(d/2 + 1)}.$$

To see the implication of Theorem 16, we proceed as follows. Consider a grid of values  $\mathcal{H} \subset (0, h_*)$  of cardinality  $n^\beta$ , for some  $0 < \beta < 1$ . By Hoeffding’s inequality, with probability at least  $1 - \frac{1}{n}$ , we have that

$$\sup_{h \in \mathcal{H}} |\Xi(h) - \mathbb{E}(\Xi(h))| \leq w_n \equiv \sqrt{\frac{2 \log(2n)(1 - \beta)}{n}}.$$

Replacing  $\mathbb{E}(\Xi(h))$  by  $\Xi(h) + w_n$  and  $\Xi(h) - w_n$  in the upper and lower bounds of part 4 of Theorem 16, respectively, setting them both equal to  $\alpha$  and then finally solving for  $h$ , we conclude that the selected  $\hat{h}$  is upper bounded by

$$h_* - \left( \frac{\alpha - w_n}{2D_1} \right)^{1/(n+1)} D_2^{-n/(n+1)}$$

and lower bounded by

$$h_* - \left( \frac{\alpha + w_n}{D_3} \right)^{1/(d(n+1))} D_4^{-n/(d(n+1))}$$

with probability larger than  $1 - \frac{1}{n}$ . Thus, as  $n \rightarrow \infty$ , the resulting bandwidth does not tend to 0. Hence, the stability based method leads to bandwidths that are quite different than the method in the previous section. Our explanation for this finding is that the stability criterion is essentially aimed at reducing the variability of the clustering solution, but it is virtually unaffected by the bias caused by large bandwidths.

In the analysis above, we assumed for simplicity that  $\lambda = 0$ . When  $\lambda > 0$ , the instability  $\Xi(h)$  can have some large peaks for very large  $h$ . This occurs when  $h$  is large enough so that some mode of  $p_h(x)$  is close to  $\lambda$ . Choosing  $h$  according to (25) will then lead to serious oversmoothing. Instead, we can choose  $\hat{h}$  as follows.

Let  $h_0 = \arg \max_h \Xi(h)$  and define

$$(26) \quad \widehat{h} = \inf\{h : h \geq h_0, \Xi(h) \leq \alpha\}.$$

We will revisit this issue in Section 6. A theoretical analysis of this modified procedure is tedious and, in the interest of space, we shall not pursue it here.

**5. Approximating the clusters.** Lemma 2 shows that, under mild conditions and when the sample size is large enough,  $N(\lambda) = \widehat{N}_h(\lambda)$  uniformly over  $h \in (0, \bar{h})$  with high probability. However, computing the number of connected components of  $\widehat{L}_h(\lambda)$  exactly is computationally difficult, especially if  $d$  is large. In this section, we study a graph-based algorithm for finding the connected components of  $\widehat{L}_h$  and for estimating the number of  $\lambda$ -clusters  $N(\lambda)$  that is based on the  $\rho$ -nearest neighborhood graph of  $\{X_i : \widehat{p}_h(X_i) \geq \lambda\}$  that is fast and easy to implement.

The idea using the union of balls of radius  $\rho$  centered at the sample points to recover certain properties of the support of a probability distribution is well understood. For instance, Devroye and Wise (1980) and Korostelev and Tsybakov (1993) use it as a simple yet effective estimator of the support, while Niyogi, Smale and Weinberger (2008) show how it can be utilized for identifying certain homology features of the support.

In particular, Cuevas, Febrero and Fraiman (2000) and Biau, Cadre and Pelletier (2007) propose to combine a kernel density estimation with a single-linkage graph algorithm to estimate the number of  $\lambda$ -clusters [see also Jang and Hendry (2007), for an application to large databases]. Our results offer similar guarantees but hold under more general settings.

The algorithm proceeds as follows. For some  $h \in (0, \bar{h})$  and a given  $\lambda \geq 0$ :

1. compute the kernel density estimate  $\widehat{p}_h$ ;
2. compute the  $\rho$ -nearest neighborhood graph of  $\{X_i : \widehat{p}_h(X_i) \geq \lambda\}$ , that is the graph  $\mathcal{G}_{h,n}$  on  $\{X_i : \widehat{p}_h(X_i) \geq \lambda\}$  where there is an edge between any two nodes if and only if they both belong to a ball of radius  $\rho$ ;
3. compute the connected components of  $\mathcal{G}_{h,n}$  using a depth-first search.

The computational complexity of the last step is linear in the number of nodes and the number of edges of  $\mathcal{G}_{h,n}$  [see, e.g., Cormen et al. (2002)], which are both random.

We will show that, if  $\rho$  is chosen appropriately, then, with high probability as  $n \rightarrow \infty$ :

1. the number of connected components of  $\mathcal{G}_{h,n}, \widehat{N}_h^G(\lambda)$ , matches the number of true clusters,  $N(\lambda) = k$ ;
2. there exists a permutation of  $\{1, \dots, k\}$  such that, for each  $j$  and  $j'$ ,

$$(27) \quad C_j^h \subseteq \bigcup_{x \in \mathcal{C}_{\sigma(j)}} B(x, \rho) \quad \text{and} \quad \left( \bigcup_{x \in \mathcal{C}_{\sigma(j)}} B(x, \rho) \right) \cap \left( \bigcup_{x \in \mathcal{C}_{\sigma(j')}} B(x, \rho) \right) = \emptyset,$$

where  $\mathcal{C}_1, \dots, \mathcal{C}_k$  are the connected components of  $\mathcal{G}_{h,n}$ .

We will assume the following regularity condition on the densities  $p_h$ , which is satisfied if the kernel  $K$  is of class  $\mathcal{C}^1$  and  $P$  is not flat in a neighborhood of  $\lambda$ :

(G) there exist constants  $\varepsilon_1 > 0$  and  $C_g > 0$  such that for each  $h \in (0, \bar{h})$ ,  $p_h$  is of class  $\mathcal{C}^1$  on  $\{x : |p_h(x) - \lambda| < \varepsilon_1\}$  and

$$(28) \quad \inf_{h \in (0, \bar{h})} \inf_{x \in \{|p_h(x) - \lambda| < \varepsilon_1\}} \|\nabla p_h(x)\| > C_g.$$

Let  $\delta_h = \min_{i \neq j} \inf_{x \in \mathcal{C}_i^h, y \in \mathcal{C}_j^h} \|x - y\|$  and set  $\delta = \inf_{h \in (0, \bar{h})} \delta_h$ . Notice that, under (C2)(b),  $\delta > 0$ . Finally, let  $\mathcal{O}_{h,n}$  denote the event in (27), which clearly implies the event  $\{\widehat{N}_h^G(\lambda) = k\}$ .

**THEOREM 17.** *Assume conditions (G) and (C2) and let  $d^* = \dim(L)$ . Assume further that there exists a constant  $\bar{C}$  such that, for every  $r \leq \delta/2$  and for  $P$ -almost all  $x \in S \cap L$ ,*

$$(29) \quad P(B(x, r)) > \bar{C}r^{d_i},$$

where  $d_i = \dim(S_i)$ , with  $x \in S_i$ . Then there exists positive constants  $\bar{\rho}$  and  $\bar{M}$ , depending on  $d^*$  and  $L$  such that, for every  $\rho < \min\{\delta/2, \bar{\rho}\}$ , there exists a number  $\varepsilon(\rho)$  such that, for any  $\varepsilon < \eta(\rho)$ ,

$$\mathbb{P}(\mathcal{O}_{h,n}^c) \leq \mathbb{P}(\mathcal{E}_{h,\varepsilon}^c) + \bar{M}\rho^{-d^*} e^{-\bar{C}n\rho^{d^*}},$$

uniformly in  $h \in (0, \bar{h})$ .

The previous result deserves few comments. First, the constants  $\bar{\rho}$ ,  $\bar{M}$  and  $\bar{C}$  depend on  $d^*$ . Second, assumption (29) is a natural generalization to lower-dimensional sets of the standardness assumption used, for example, in Cuevas and Fraiman (1997). It is clearly true for components  $P_i$  of full-dimensional support that are absolutely continuous with respect to the Lebesgue measure. Finally, in view of Lemma 19 [and, specifically, of the way  $\varepsilon(\rho, \tau)$  is defined], Theorem 17 holds for sequences  $\{\varepsilon_n\}$ ,  $\{h_n\}$  and  $\{\rho_n\}$  such that:

1.  $\varepsilon_n = o(1)$ ,
2.  $\sup_n h_n \leq \bar{h}$ ;
3.  $\sup_n \rho_n < \min\{\delta/2, \bar{\rho}_d\}$  and  $\varepsilon_n = o(\rho_n)$ .

In particular, if  $h_n = o(1)$ , then, following Proposition 9, the term  $\mathbb{P}(\mathcal{E}_{h_n, \varepsilon_n}^c)$  vanishes if  $\frac{nh_n^{d^*}}{|\log h_n^{d^*}|} \rightarrow \infty$ . Interestingly enough, condition (C1) does not play a direct role in Theorem 17.

We now consider a bootstrap extension of the previous algorithm, as suggested in Cuevas, Febrero and Fraiman (2000). For any  $h$ , let  $X^* = (X_1^*, \dots, X_N^*)$ , denote a bootstrap sample from  $\widehat{p}_h$  conditionally on  $\{\widehat{p}_h \geq \lambda\}$  and let  $\mathcal{G}_{n,h}^*$  denote the  $\rho$ -

neighborhood graph with node set  $X^*$ . Finally, let  $\mathcal{O}_{h,n}^*$  be the event given in (27), except that  $\mathcal{C}_1, \dots, \mathcal{C}_k$  are now the connected components of  $\mathcal{G}_{h,n}^*$ .

**THEOREM 18.** *Assume conditions (C2) and (G). Suppose that there exist positive constants  $\bar{C}$  and  $\bar{\rho}$  such that*

$$(30) \quad \inf_{h \in (0, \bar{h})} \int_{A_h \cap L_h(\lambda)} p_h d\mu > \bar{C} \rho^d$$

for any ball  $A_h$  of radius  $\rho < \bar{\rho}$  and center in  $L_h(\lambda)$ . Then, for any  $\rho \leq \min\{\delta/2, \bar{\rho}\}$ , there exists a positive number  $\varepsilon(\rho)$  such that, for each  $\varepsilon < \varepsilon(\rho)$ ,

$$\mathbb{P}((\mathcal{O}_{h,n}^*)^c) \leq \mathbb{P}(\mathcal{E}_{h,\varepsilon}^c) + \bar{M} \rho^{-d} e^{-CN\rho^d},$$

uniformly in  $h \in (0, \bar{h})$ , where  $\bar{M}$  and  $C$  are positive constants independent of  $h$  and  $\rho$ .

The constants  $C, \bar{C}, \bar{\rho}$ , and  $\bar{M}$  depend on both  $d$  and  $S \oplus B(0, \bar{h})$ . In our settings, condition (30) clearly holds if  $P$  has full-dimensional support. More generally, it can be shown that conditions (G) and (29) imply (30).

Just like with Theorem 17, using Lemma 19, it can be verified that the theorem holds if one consider sequences of parameters depending on the sample size such that  $\varepsilon_n = o(1)$ ,  $\varepsilon_n = o(\rho_n)$ ,  $\sup_n \rho_n < \max\{\delta/2, \bar{\rho}\}$  and  $\sup_n h_n < \bar{h}$ , provided that the conditions of Proposition 9 are met.

Despite the similar form for the error bounds of Theorems 17 and 18, there are some marked differences. In fact, in Theorem 17 the performance of the algorithm depends directly on the sample size  $n$  and, in particular, on the actual dimension  $d^* \leq d$  of the support of  $P$ , with smaller values of  $d^*$  yielding better guarantees. In contrast, besides  $n$ , the performance of the algorithm based on the bootstrap sample depends on the ambient dimension  $d$ , regardless of  $d^*$ , and on the bootstrap sample size  $N$ . By choosing  $N$  very large, the expression  $\mathbb{P}(\mathcal{E}_{h,\varepsilon}^c)$  becomes the leading term in the upper bound of the probability of the event  $(\mathcal{O}_{h,n}^*)^c$ .

**6. Examples.** In this section, we consider a few examples to illustrate the methods.

6.1. *A one dimensional example.* In Section 4.2, we pointed out that when  $\lambda > 0$  and large, it is safer to use the modified rule  $\hat{h} = \inf\{h : h \geq h_0, \Xi(h) \leq \alpha\}$  where  $h_0 = \arg \max_h \Xi(h)$ , in place of the original rule  $\hat{h} = \inf\{h : \sup_{t>h} \Xi(t) \leq \alpha\}$ . We illustrate this with a simple one-dimensional example.

Figure 3 shows an example based on  $n = 200$  points from the density  $p$  that is uniform on  $[0, 1] \cup [5, 6]$ . When  $\lambda = 0$  (top), the original rule works fine. (We use  $\alpha = 0.05$ .) The selected bandwidth is small leading to the very wiggly density estimator in the top right plot. However, this estimator correctly estimates the level

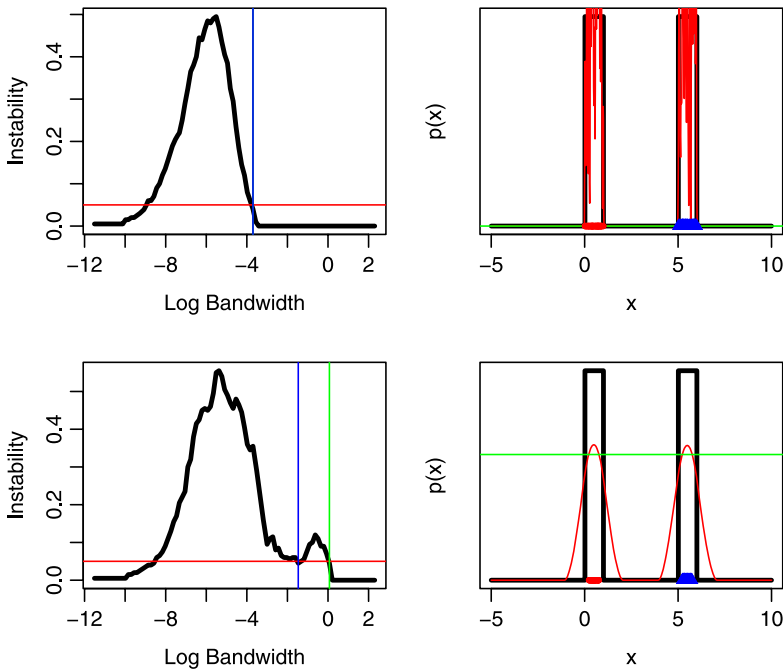


FIG. 3. The left plots show the instability as a function of log bandwidth. The horizontal line shows  $\alpha = 0.05$ . The right plots show the true density and the kernel density estimator based on the selected bandwidth  $h$ . In the top plots,  $\lambda = 0$ . In the bottom plots,  $\lambda = 0.3$ .

set and the clusters. In the bottom, we have  $\lambda = 0.3$ . When  $h$  is large, there is a blip in the instability curve corresponding to the fact that the modes of  $p_h(x)$  are close to  $\lambda$ . The original rule corresponds to the second vertical line in the bottom left plot. The resulting density estimator shown in the bottom right plot is oversmoothed and leads to no points being in the set  $\hat{p}_h \geq \lambda$ . The modified rule corresponds to the first vertical line in the bottom left plot. This bandwidth works fine.

Figure 4 compares the instability method (top) with the excess mass method (bottom). Both methods recover the level set and the clusters. We took  $\lambda = 0.3$  in both cases. Because  $\lambda$  is very large, the excess mass becomes undefined for large  $h$  since  $p_h(x) < \lambda$  for all  $x$ , which we denoted by setting the risk to 0 in the bottom left plot.

6.2. *Fuzzy stick with spiral.* Figure 5 shows data from a fuzzy stick with a spiral. The stick has noise while the spiral is supported on a lower-dimensional curve. Figure 6 shows the clusterings from the instability method and the excess risk method with  $\lambda = 0$ . Both recover the clusters perfectly. Note that the excess risk is necessarily equal to 1 for large  $h$ . In this case, we take  $\hat{h}$  to be the smallest



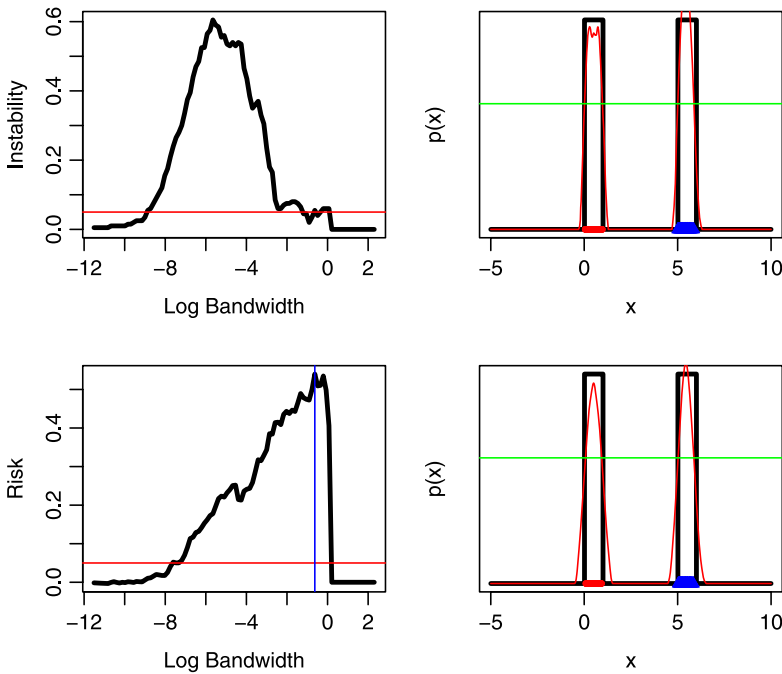


FIG. 4. The top left plot shows the instability as a function of log bandwidth. The top right plot shows the true density and the kernel density estimator based on the selected bandwidth  $h$  using the modified rule. The bottom left plot shows the estimated excess mass risk as a function of log bandwidth. The top right plot shows the true density and the kernel density estimator based on the selected bandwidth  $h$  obtained by maximizing the excess mass. In both bottom plots,  $\lambda = 0.3$ . Both methods recover the level set and the clusters.

$h$  of all bandwidths that maximize the excess mass. We see that both methods recover the clusters.

6.3. *Two moons.* This is a 20-dimensional example. The data lie on two half-moons embedded in  $\mathbb{R}^{20}$ . The results are shown in Figure 7. Only the first two coordinates of the data are plotted. Again we see that both methods recover the clusters.

**7. Discussion.** As is common in density clustering, we have assumed a fixed, given value of  $\lambda$ . In practice, we recommend that the results should be computed for a range of values of  $\lambda$  [see, e.g., Stuetzle and Nugent (2010), and references therein]. It is important to choose a different bandwidth for each  $\lambda$ . Indeed, inspection of the proof of Theorem 12 shows that the optimal bandwidth is a function of  $\lambda$  and that  $h(\lambda) \rightarrow 0$  as  $\lambda$  increases. Further research on data-dependent methods to choose  $\lambda$  and  $\rho$  (the parameter used in the graph-based algorithm of Section 5) would be very useful.

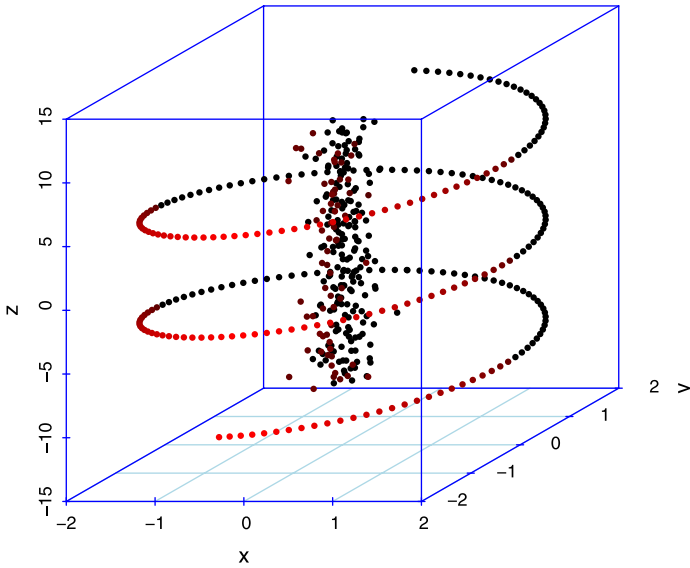


FIG. 5. 500 data points from a fuzzy stick plus a spiral.

We discussed the idea of using stability to choose a bandwidth. We saw that the behavior of the selected bandwidth is quite different than with the excess mass method. This method seems to work well for density clustering unlike what happens for  $k$ -means clustering [Ben-David, von Luxburg and Pall (2006)]. We believe

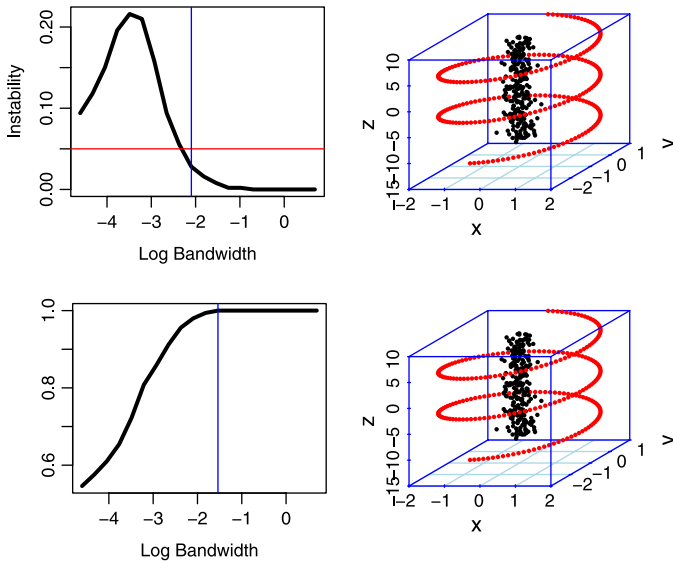


FIG. 6. Clusters obtained from instability (top) and excess mass (bottom).

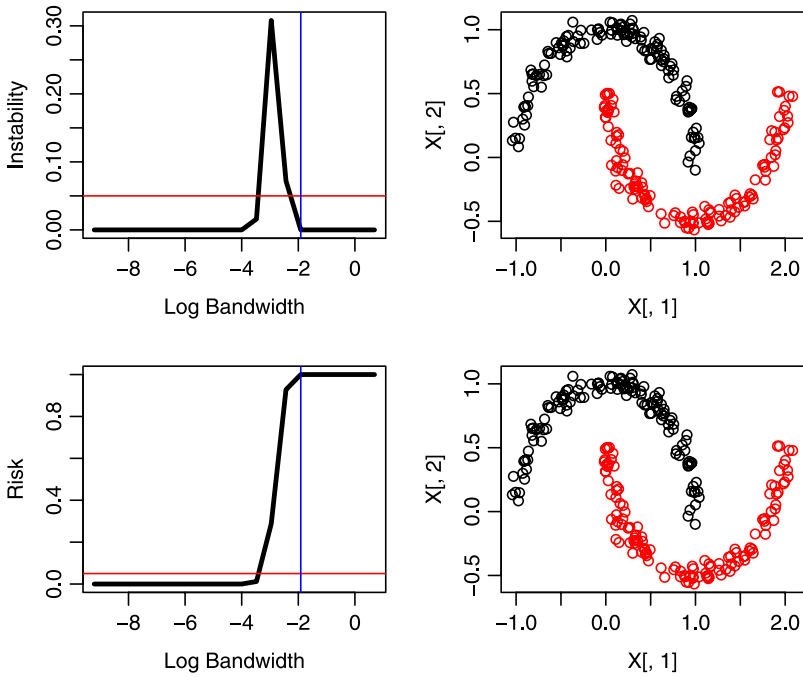


FIG. 7. Clusters obtained from instability (top) and excess mass (bottom). The data are in  $\mathbb{R}^{20}$  but only the first two components are plotted.

that the stability method deserves more scrutiny. In particular, it would be helpful to understand the behavior of the stability measure under more general conditions. Also, the detailed theoretical properties of the modified method for selecting  $h$  based on stability should be explored.

Finally, we note that there is growing interest in spectral clustering methods [von Luxburg (2007)]. We believe there are connections between the work reported here and spectral methods.

**8. Proofs.** PROOF OF LEMMA 1. The weak convergence follows from the fact that  $P$  is a Radon measure [see, e.g., Leoni and Fonseca (2007), Theorem 2.79]. As for the second part, if  $x \in S_i$ , where  $S_i$  has Hausdorff dimension  $d$ , then  $p(x) = \pi_i p_i(x)$ , with  $p_i$  a Lebesgue density, and the result follows directly from Leoni and Fonseca (2007), Theorem 2.73, part (ii). See also the Appendix. On the other hand if  $d_i < d$ , then it is necessary to modify the arguments as follows. Since  $K$  is smooth and supported on  $B(0, 1)$ , there exists a  $\eta$  such that  $K(\frac{x-y}{h}) > \eta$  if  $\|x - y\| < \eta h$ . Set  $C = \frac{\eta^{d_i+1} v_{d_i}}{c_d}$ , where  $v_{d_i}$  is the volume of the unit Euclidean

ball in  $\mathbb{R}^{d_i}$ . Then

$$\begin{aligned} p_h(x) &= \frac{1}{c_d h^d} \int_{S_i \cap B(x, h)} K\left(\frac{x-y}{h}\right) dP(y) \\ &\geq \frac{1}{c_d h^d} \eta \int_{S_i \cap B(x, \eta h)} dP(y) \\ &= \frac{\eta^{d_i+1} v_{d_i}}{c_d h^{d-d_i}} \frac{1}{v_{d_i} (\eta h)^{d_i}} P_i(B(x, \eta h)) \\ &= \frac{C}{h^{(d-d_i)}} \frac{P_i(B(x, \eta h))}{v_{d_i} (\eta h)^{d_i}}. \end{aligned}$$

As  $h \rightarrow 0$ ,  $\frac{P_i(B(x, \eta h))}{v_{d_i} (\eta h)^{d_i}} \rightarrow p_i(x) < \infty$ , by (39) almost everywhere  $\mathcal{H}^{d_i}$ , while  $\frac{C}{h^{(d-d_i)}} \rightarrow \infty$ , thus showing that  $\lim_{h \rightarrow 0} p_h(x) = \infty$ .  $\square$

**PROOF OF LEMMA 2.** By assumption (C2), for any  $0 \leq \varepsilon < \bar{\varepsilon}$  and  $0 < h < \bar{h}$ ,

$$N_h(\lambda - \varepsilon) = N_h(\lambda) = N_h(\lambda + \varepsilon) = N(\lambda) = k.$$

On the event  $\mathcal{E}_{h, \varepsilon}$  it holds that

$$L_h(\lambda + \|p_h - \hat{p}_h\|_\infty) \subseteq \hat{L}_h(\lambda) \subseteq L_h(\lambda - \|p_h - \hat{p}_h\|_\infty),$$

which implies that, on the same event,

$$k = N_h(\lambda + \|p_h - \hat{p}_h\|_\infty) \leq \hat{N}_h(\lambda) \leq N_h(\lambda - \|p_h - \hat{p}_h\|_\infty) = k. \quad \square$$

**PROOF OF LEMMA 3.** Recall that  $K_h$  is supported on  $B(0, h)$ . For the first claim, it is enough to show that, for any  $\varepsilon \in [0, \bar{\varepsilon}]$ ,  $L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon) \subseteq \partial L(\lambda - \varepsilon) + B(0, h)$ . Indeed, by (C3),  $\mu(\partial L(\lambda - \varepsilon) \oplus B(0, h)) \leq C_2 h^\theta$ , which implies (10). Thus, we will prove that, if  $w \notin \partial L(\lambda - \varepsilon) \oplus B(0, h)$ , then  $w \notin L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)$ . For such a point  $w$ , either  $p(w) \geq \lambda - \varepsilon$  or, by conditions (C2),  $p(z) < \lambda - \varepsilon$  for every  $z \in B(w, h)$ . Since the kernel  $K$  has compact support, the latter case implies that  $p_h(w) < \lambda - \varepsilon$  as well. Therefore,

$$\begin{aligned} w &\in \{x : p(x) \geq \lambda - \varepsilon\} \cup \{x : p_h(x) < \lambda - \varepsilon\} \\ &= \{x : p(x) < \lambda - \varepsilon, p_h(x) \geq \lambda - \varepsilon\}^c \\ &= (L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon))^c. \end{aligned}$$

As for inequality (11), it is enough to observe that the set

$$I_{h, \varepsilon} = (L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \cap S$$

either has zero probability (because it is empty or has Lebesgue measure 0) or has positive Lebesgue measure. In the former case, we obtain  $\xi = \infty$ . In the latter case,

$I_{h,\varepsilon}$  must be full dimensional, so that, by (10),  $\mu(I_{h,\varepsilon}) \leq C_3h$ , for all  $h \in (0, \bar{h})$ . Since  $p$  is bounded by  $\lambda$  on  $I_{h,\varepsilon}$ , we obtain

$$P(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) = P(I_{h,\varepsilon}) \leq \lambda C_2h = C_3h,$$

which implies that we can take  $\xi = 1$ .  $\square$

PROOF OF LEMMA 4. Since  $p$  is Lipschitz and integrable,  $p^{-1}(\lambda)$  is  $\mathcal{H}^{d-1}$ -measurable, so the integral  $\mathcal{H}^{d-1}(\{x : p(x) = \lambda\})$  is well defined for  $\lambda \in (0, \|p\|_\infty)$ , where  $\mathcal{H}^{d-1}$  denote the  $(d - 1)$ -dimensional Hausdorff measure in  $\mathbb{R}^d$ . Furthermore, we can use the coarea formula. See Evans and Gariepy (1992) and Ambrosio, Fusco and Pallara (2000) for backgrounds on Hausdorff measures and the coarea formula. By the Rademacher theorem, the set  $E_1$  of points where  $p$  is not differentiable has Lebesgue measure zero. By Lemma 2.96 in Ambrosio, Fusco and Pallara (2000), the set  $E_2 = \{x : \|\nabla p(x)\| = 0\}$  is such that  $\mathcal{H}^{d-1}\{p^{-1}(\lambda) \cap E_2\} = 0$ , for all  $\lambda \in (0, \|p\|_\infty)$  outside of a set  $E_3 \subset \mathbb{R}$  of Lebesgue measure 0. Without loss of generality, below we may assume that  $E_1$  and  $E_2$  are empty. Thus, we can assume that, for any  $\lambda \in (0, \|p\|_\infty) \cap E_3^c$ , there exists positive numbers  $\bar{\varepsilon}$ ,  $C$  and  $M$  such that:

- (i)  $\inf_{x \in \{x : |p(x) - \lambda| < \bar{\varepsilon}\}} \|\nabla p(x)\| > C$ , almost everywhere- $\mu$ ;
- (ii)  $\sup_{\eta \in (-\bar{\varepsilon}, \bar{\varepsilon})} \mathcal{H}^{d-1}(\{x : p(x) = \lambda + \eta\}) < M$ .

Then for each  $\varepsilon \in (0, \bar{\varepsilon})$ ,

$$\begin{aligned} P(\{x : |p(x) - \lambda| < \varepsilon\}) &= \int p(x) 1_{\{|p(x) - \lambda| < \varepsilon\}} d\mu(x) \\ &= \int \frac{p(x)}{\|\nabla p(x)\|} 1_{\{|p(x) - \lambda| < \varepsilon\}} \|\nabla p(x)\| d\mu(x) \\ &= \int_{-\varepsilon}^{+\varepsilon} \int_{\{p^{-1}(\lambda+u)\}} \frac{p(x)}{\|\nabla p(x)\|} d\mathcal{H}^{n-1}(x) du \\ &= \int_{-\varepsilon}^{+\varepsilon} (\lambda + u) \int_{\{p^{-1}(\lambda+u)\}} (\|\nabla p(x)\|)^{-1} d\mathcal{H}^{n-1}(x) du \\ &\leq \frac{2\lambda M}{C} \varepsilon, \end{aligned}$$

where the second equality holds because  $\|\nabla p(x)\|$  is bounded away from 0 on  $\{x : |p(x) - \lambda| < \varepsilon\}$  by (i), the third equality is a direct application of the coarea formula [see, e.g., Proposition 3, page 118 in Evans and Gariepy (1992)] and the last inequality follows from (i) and (ii).  $\square$

PROOF OF COROLLARY 5. Following the proof of Lemma 4 and using our additional assumption that  $p$  is of class  $\mathcal{C}^1$ , without any loss of generality, below

we can assume that the set  $E_1$  and  $E_2$  are empty and we recall that  $E_3$  has Lebesgue measure 0. Let  $\lambda \notin E_3$  be such that

$$\inf_{x \in p^{-1}(\lambda)} \|\nabla p(x)\| > 0.$$

We now claim that there exists a nonempty neighborhood  $U$  of  $\lambda$  for which

$$\inf_{\lambda \in U} \inf_{x \in p^{-1}(\lambda)} \|\nabla p(x)\| > 0.$$

Indeed, arguing by contradiction, suppose that the previous display were not verified for any neighborhood  $U$  of  $\lambda$ . Then there exist sequences  $\{\lambda_n\} \subset \mathbb{R}$  and  $\{x_n\} \subset S$  such that  $\lim_n \lambda_n = \lambda$ , and  $x_n \in p^{-1}(\lambda_n)$  and  $\nabla p(x_n) = 0$  for each  $n$ . By compactness, it is possible to extract a subsequence  $\{x_{n_k}\}$  of  $\{x_n\}$  such that  $x_{n_k} \rightarrow x$ , for some  $x \in p^{-1}(\lambda)$ . Since  $p$  is of class  $\mathcal{C}^1$ , this implies that  $\nabla p(x_{n_k}) \rightarrow \nabla p(x)$  as well. However,  $\nabla p(x_{n_k}) = 0$  for each  $k$  by construction, while  $\nabla p(x) \neq 0$ . This produces a contradiction. Thus, for each  $\lambda$  that is not a critical point, one can find a neighborhood of positive length containing it and, by Lemma 4, (C1) holds at  $\lambda$  with  $\gamma = 1$ . Since, using compactness again,  $\|p\|_\infty < \infty$ , this implies that there can only be a finite number of critical points for which  $\gamma$  may differ from 1.  $\square$

PROOF OF LEMMA 8. Since  $\varepsilon < \bar{\varepsilon}$  and  $h < \bar{h}$ , in virtue of (C2)(b) it holds that, on  $\mathcal{E}_{h,\varepsilon}$ ,

$$\widehat{L}_h(\lambda) \supseteq L_h(\lambda + \varepsilon) \supseteq L(\lambda + \varepsilon)$$

and

$$\widehat{L}_h(\lambda) \subseteq L_h(\lambda - \varepsilon) = L(\lambda - \varepsilon) \cup (L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)).$$

Because  $L(\lambda + \varepsilon) \subseteq L(\lambda) \subseteq L(\lambda - \varepsilon)$ , the above inclusions imply, still on  $\mathcal{E}_{h,\varepsilon}$ , that

$$\begin{aligned} \widehat{L}_h(\lambda) \Delta L(\lambda) &\subseteq (L(\lambda - \varepsilon) - L(\lambda + \varepsilon)) \cup (L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \\ &= A \cup B, \end{aligned}$$

where it is clear that the sets  $A$  and  $B$  are disjoint. Taking expectation with respect to  $P$  of the indicators of the sets  $\widehat{L}_h(\lambda) \Delta L(\lambda)$ ,  $A$  and  $B$  and using condition (C1) and Lemma 3 yield (14).  $\square$

PROOF OF PROPOSITION 9. The claimed results are a direct consequence of Corollary 2.2 in Giné and Guillou (2002). We outline the details below. We rewrite the left-hand side of (17) as

$$\mathbb{P} \left\{ \left\| \sum_{i=1}^n f(X_i) - \mathbb{E}[f(X_1)] \right\|_{\mathcal{F}_h} > 2\varepsilon nh^d \right\},$$

where

$$\mathcal{F}_h = \left\{ K\left(\frac{x - \cdot}{h}\right), x \in \mathbb{R}^d \right\}$$

and then proceed to apply Giné and Guillou (2002), Corollary 2.2. Following their notation, we set  $t = nh^d \varepsilon$  and, since,

$$\sup_{f \in \mathcal{F}_h} \text{Var}[f] \leq \sup_z \int_{\mathbb{R}^d} K^2\left(\frac{z - x}{h}\right) dP(x) \leq h^d D,$$

we can further take  $\sigma^2 = h^d D$  and  $U = C \|K\|_\infty$ , where  $C$  is a positive constant, depending on  $h$ , such that  $\sigma < U/2$ . Then conditions (2.4), (2.5) and (2.6) of Giné and Guillou (2002) are satisfied for all  $n$  bigger than some finite  $n_0$ , which depends on the VC characteristics of  $K$ ,  $D$ ,  $\|K\|_\infty$ ,  $C$  and  $\varepsilon$ . Part 2 is proved in a very similar way. In this case, we take the supremum over the the entire class  $\mathcal{F}$  and we set  $\sigma_n^2 = h_n^d D$  and  $U = \|K\|_\infty$ . For all  $n$  large enough, condition (2.5) is trivially satisfied because  $h_n = o(1)$ , while equations (2.4) and (2.6) hold true by virtue of (18). The unspecified constants again depend on the VC characteristics of  $K$ ,  $D$  and  $\|K\|_\infty$ .  $\square$

PROOF OF THEOREM 10. We can write

$$(31) \quad \mathbb{E}(\rho(p, \hat{p}_h, P)) = \mathbb{E}\left(\int_{\hat{L}_h(\lambda) \Delta L(\lambda)} dP; \mathcal{E}_{h,\varepsilon}\right) + \mathbb{E}\left(\int_{\hat{L}_h(\lambda) \Delta L(\lambda)} dP; \mathcal{E}_{h,\varepsilon}^c\right),$$

where for a random variable  $X$  defined on some probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and an event  $\mathcal{E} \subset \mathcal{F}$ ,  $\mathbb{E}(X; \mathcal{E}) \equiv \int_{\Omega \cap \mathcal{E}} X(\omega) d\mathbb{P}(\omega)$ . Using Proposition 9, the second term on the right-hand side is upper bounded by

$$(32) \quad \mathbb{P}(\mathcal{E}_{h,\varepsilon}) \leq L e^{-nC_K h^d \varepsilon^2}.$$

As for the first term on the right-hand side of (31), without loss of generality, we consider separately the case in which the support of  $P$  has no lower-dimensional components and the case in which it of lower dimension. The result for the cases in which the support has components of different dimensions follows in a straightforward way.

If the support of  $P$  consists of full-dimensional sets, then, on the event  $\mathcal{E}_{h,\varepsilon}$ ,

$$\begin{aligned} \int_{\hat{L}_h(\lambda) \Delta L(\lambda)} dP &\leq P(L(\lambda - \varepsilon) - L(\lambda + \varepsilon)) + P(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \\ &\leq C_1 \varepsilon^\gamma + C_3 h^\xi, \end{aligned}$$

where the first inequality stems from (14) and the second from conditions (C1) and (11).

If instead  $P$  has lower-dimensional support, then, because, on the event  $\mathcal{E}_{h,\varepsilon}$ ,  $\hat{L}_h \subset L_h(\lambda - \varepsilon)$  and because  $L \subset L_h(\lambda - \varepsilon)$  by (C2)(b), we see that, on  $\mathcal{E}_{h,\varepsilon}$ ,

$$\int_{\hat{L}_h(\lambda) \Delta L(\lambda)} dP = 0.$$

We conclude that  $\mathbb{E}(\rho(p, \widehat{p}_h, P); \mathcal{E}_{h,\varepsilon})$  is bounded by  $\max\{C_1, C_3\}(\varepsilon^\gamma + h^\xi)$  if the support of  $P$  contains a full-dimensional set and is 0 otherwise. This, combined with (32), yields the claimed upper bound on the level set risk with  $C_L = \max\{C_1, C_3, L\}$ . The convergence rates are established using simple algebra. Notice that the choice of the sequences  $\{\varepsilon_n\}$  and  $\{h_n\}$  does not violate condition (18).  $\square$

PROOF OF COROLLARY 11. For each  $i \in \{1, \dots, n\}$ ,

$$\mathbb{P}(i \in \widehat{I}_h | \mathcal{E}_{h,\varepsilon}) \leq \mathbb{P}(X_i \in \widehat{L}_h \Delta L | \mathcal{E}_{h,\varepsilon}) \leq \max\{C_1, C_3\}(\varepsilon^\gamma + h^\xi) \frac{1}{\mathbb{P}(\mathcal{E}_{h,\varepsilon})},$$

where the last inequality is due to Lemma 8. Thus,

$$\begin{aligned} \mathbb{E}(|\widehat{I}_h|) &\leq \sum_{i=1}^n \mathbb{P}(i \in \widehat{I} | \mathcal{E}_{h,\varepsilon}) \mathbb{P}(\mathcal{E}_{h,\varepsilon}) + n \mathbb{P}(\mathcal{E}_h^c) \\ &\leq n(\max\{C_1, C_3\}(\varepsilon^\gamma + h^\xi) + \mathbb{P}(\mathcal{E}_h^c)) \\ &\leq C_L(\varepsilon^\gamma + h^\xi + e^{-C_K n h^d \varepsilon^2}). \end{aligned} \quad \square$$

PROOF OF THEOREM 12. From (9), we have

$$\mathcal{E}(L) - \mathcal{E}(\widehat{L}_h) = \int_{\widehat{L}_h \Delta L} |p_0 - \lambda| d\mu + P_1(L) - P_1(\widehat{L}_h),$$

where  $p_0 = \frac{dP_0}{d\mu}$ . Since, on the event  $\mathcal{E}_{h,\varepsilon}$ ,  $\widehat{L}_h \supset L_h(\lambda + \varepsilon)$ , we obtain, on the same event,

$$P_1(L) - P_1(\widehat{L}_h) \leq P_1(L) - P_1(L_h + \varepsilon) = 0,$$

where the last equality is due to condition (C2)(b). Therefore,

$$\mathcal{E}(L) - \mathcal{E}(\widehat{L}_h) \leq \int_{\widehat{L}_h \Delta L} |p_0 - \lambda| d\mu.$$

Just like in the proof of Theorem 10, we treat separately the case in which the support of  $P$  is of lower-dimension and the case in which it consists of full-dimensional sets. If the support of  $P$  is not of full dimension, then, on  $\mathcal{E}_{h,\varepsilon}$ ,

$$\mathcal{E}(L) - \mathcal{E}(\widehat{L}_h) \leq \lambda \mu(\widehat{L}_h \Delta L) \leq \lambda \mu(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \leq \lambda C_2 h^\theta$$

by (10). On the other hand, if the support of  $P$  has no lower-dimensional components (so that  $p_0 = p$ ), still on the event  $\mathcal{E}_{h,\varepsilon}$  and using Lemma 8,

$$(33) \quad \begin{aligned} \int_{\{\widehat{L}_h(\lambda) \Delta L(\lambda)\}} |p - \lambda| d\mu &\leq \int_{L(\lambda - \varepsilon) - L(\lambda + \varepsilon)} |p - \lambda| d\mu \\ &\quad + \int_{L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)} |p - \lambda| d\mu. \end{aligned}$$



The first term on the right-hand side of the previous inequality can be bounded as follows:

$$\begin{aligned} \int_{L(\lambda-\varepsilon)-L(\lambda+\varepsilon)} |p - \lambda| d\mu(x) &= \int_{\{x: |p(x)-\lambda|<\varepsilon\}} |p - \lambda| d\mu(x) \\ &\leq \varepsilon \int_{\{x: |p(x)-\lambda|<\varepsilon\}} d\mu(x) \\ &= \frac{\varepsilon}{\lambda - \varepsilon} \int_{\{x: |p(x)-\lambda|<\varepsilon\}} (\lambda - \varepsilon) d\mu \\ &\leq \frac{\varepsilon}{\lambda - \varepsilon} \int_{\{x: |p(x)-\lambda|<\varepsilon\}} p(x) d\mu(x) \\ &\leq \frac{C_1}{\lambda - \varepsilon} \varepsilon^{\gamma+1}, \end{aligned}$$

where the last inequality is due to condition (C1). As for the second term of the right-hand side of (33),

$$\int_{L_h(\lambda-\varepsilon)-L(\lambda-\varepsilon)} |p - \lambda| d\mu \leq \lambda\mu(L_h(\lambda - \varepsilon) - L(\lambda - \varepsilon)) \leq \lambda C_2 h^\theta$$

by (10).

Thus, we conclude that  $\mathbb{E}(\mathcal{E}(L) - \mathcal{E}(\widehat{L}_h); \mathcal{E}^{h,\varepsilon})$  is bounded by  $\lambda C_2 h^\theta$  if the support of  $P$  is a lower-dimensional set and by

$$\max\left\{\lambda C_2, \frac{C_1}{\lambda - \varepsilon}\right\}(\varepsilon^{\gamma+1} + h^\theta)$$

otherwise. Next, by compactness of  $S$ , and using (32),

$$\mathbb{E}(\mathcal{E}(L) - \mathcal{E}(\widehat{L}_h); \mathcal{E}_{h,\varepsilon}^c) \leq (1 + \lambda\mu(S + B(0, \bar{h})))\mathbb{P}(\mathcal{E}_{h,\varepsilon}) \leq C_S(1 + \lambda)L e^{-n C_K h^d \varepsilon^2}$$

for some positive constant  $C_S$ , uniformly in  $h < \bar{h}$ . The claimed upper bound on the excess mass risk now follows by taking  $C_M = \max\{\lambda C_2, \frac{C_1}{\lambda - \varepsilon}, C_S(1 + \lambda)L\}$ . The convergence rates can be easily obtained by simple algebra. Notice that the choice of the sequences  $\{\varepsilon_n\}$  and  $\{h_n\}$  does not violate condition (18).  $\square$

**PROOF OF THEOREM 14.** This follows by combining the version of Talagrand’s inequality for empirical processes as given in Massart (2000) with an adaptation of the arguments used in the proof of Theorem 7.1 in Györfi et al. (2002). For completeness, we provide the details.

Define  $\widehat{h} = \arg \sup_{h \in \mathcal{H}} \widehat{\mathcal{E}}(L_h)$ , where

$$\widehat{\mathcal{E}}(L_h) = \frac{1}{n} \sum_{i=1}^n I(Z_i \in L_h) - \lambda\mu(L_h)$$

and  $h_* = \arg \sup_{h \in \mathcal{H}} \mathcal{E}_X(L_h)$ . Set  $\Gamma(h) = \mathcal{E}_X(L_{h_*}) - \mathcal{E}_X(L_h)$ , where  $h \in \mathcal{H}$ . Recall that both  $L_{h_*}$  and  $L_h = \{x: \widehat{p}_h \geq \lambda\}$ , are random sets depending on the training

set  $X$ . We will bound  $\mathbb{E}(\Gamma(\widehat{h}))$ , where the expectation is over the joint distribution of  $X$  and  $Y$ .

We can write

$$\mathbb{E}(\Gamma(\widehat{h})|X) = \underbrace{\mathbb{E}(\Gamma(\widehat{h})|X)}_{T_1} - \underbrace{(1 + \delta)\widehat{\Gamma}(\widehat{h})}_{T_2} + \underbrace{(1 + \delta)\widehat{\Gamma}(\widehat{h})}_{T_2},$$

where  $\widehat{\Gamma}(h) = \widehat{\mathcal{E}}(L_{h_*}) - \widehat{\mathcal{E}}(L_h)$ . Note that

$$\widehat{\Gamma}(\widehat{h}) = \widehat{\mathcal{E}}(L_{\widehat{h}}) - \widehat{\mathcal{E}}(L_{h_*}) \leq \widehat{\mathcal{E}}(L_{h_*}) - \widehat{\mathcal{E}}(L_{h_*}) = 0.$$

Thus,  $\mathbb{E}(T_2|X) \leq 0$ . We conclude that

$$(34) \quad \mathbb{E}(\Gamma(\widehat{h})) = \mathbb{E}(\mathbb{E}(\Gamma(\widehat{h})|X)) = \mathbb{E}(\mathbb{E}(T_1|X)) + \mathbb{E}(\mathbb{E}(T_2|X)) \leq \mathbb{E}(\mathbb{E}(T_1|X)).$$

Now we bound  $\mathbb{E}(T_1|X)$ . Consider the empirical process

$$Z = \sup_{h \in \mathcal{H}} \widehat{\Gamma}(h),$$

so that  $Z = \widehat{\Gamma}(\widehat{h})$  and  $\mathbb{E}(\Gamma(\widehat{h})|X) = \mathbb{E}(Z|X)$ . We have

$$\begin{aligned} \mathbb{P}(T_1 \geq s|X) &= \mathbb{P}(\mathbb{E}(Z|X) - (1 + \delta)Z \geq s | X) \\ &= \mathbb{P}\left(\mathbb{E}(Z|X) - Z \geq \frac{s + \delta\mathbb{E}(Z|X)}{1 + \delta} \mid X\right). \end{aligned}$$

Notice that, conditionally on  $X$ ,  $Z = \frac{1}{n} \sup_{h \in \mathcal{H}} \sum_{i=1}^n f_h(Y_i)$ , where, for each  $h \in \mathcal{H}$ ,  $f_h : \mathbb{R}^d \mapsto \mathbb{R}$  is the function given by

$$f_h(x) = I(x \in L_{h_*}) - \lambda\mu(L_{h_*}) - (I(x \in L_h) - \lambda\mu(L_h))$$

with  $\|f_h\|_\infty < \kappa$ . Let  $\sigma^2 \equiv \mathbb{E}(\frac{1}{n} \sup_{h \in \mathcal{H}} \sum_{i=1}^n f_h^2(Y_i)|X)$  and notice that  $\sigma^2 \leq \kappa \mathbb{E}(\sup_h \widehat{\Gamma}(h)|X) = \kappa \mathbb{E}(Z|X)$ . Thus,

$$\mathbb{P}(T_1 \geq s|X) \leq \mathbb{P}\left(\mathbb{E}(Z|X) - Z \geq \frac{s + \delta\sigma^2/\kappa}{1 + \delta} \mid X\right),$$

which, by Corollary 13 in [Massart \(2000\)](#), is upper bounded by

$$2 \exp\left\{-\frac{n((s + \delta\sigma^2/\kappa)/(1 + \delta))^2}{4(4\gamma^2\sigma^2 + 7/4\kappa\varepsilon)}\right\}.$$

Then, some algebra [see Problem 7.1 in [Györfi et al. \(2002\)](#)] yields the final bound

$$\mathbb{P}(T_1 \geq s|X) \leq 2 \exp\left\{\frac{-ns}{d(\delta, \kappa)}\right\},$$

where  $d(\delta, \kappa)$  is given in the statement of the theorem.

Set  $u = \frac{d(\delta, \kappa)}{n} \log 2$ . Then

$$\begin{aligned} \mathbb{E}(T_1|X) &= \int_0^\infty \mathbb{P}(T_1 > s|X) ds \leq u + \int_u^\infty \mathbb{P}(T_1 > s|X) ds \\ &= u + \frac{2d(\delta, \kappa)}{n} \exp\left\{-\frac{nu}{d(\delta, \kappa)}\right\} \\ &= d(\delta, \kappa) \frac{1 + \log 2}{n}. \end{aligned}$$

From (34), we conclude that

$$\mathbb{E}(\Gamma(\widehat{h})) \leq d(\delta, \kappa) \frac{1 + \log 2}{n}$$

and so

$$\mathbb{E}(M(\widehat{h})) \leq \mathbb{E}(M(h_*)) + d(\delta, \kappa) \frac{1 + \log 2}{n},$$

which implies that

$$\mathbb{E}(\mathcal{E}(\widehat{h})) \geq \mathbb{E}(\mathcal{E}(h_*)) - d(\delta, \kappa) \frac{1 + \log 2}{n}.$$

This shows (23).

**PROOF OF THEOREM 15.** Define  $r_n(\gamma, \theta) = \left(\frac{\log n}{n}\right)^{\theta(\gamma+1)/(2\theta+d(\gamma+1))}$ . For each  $\theta$ ,  $r_n(\gamma, \theta)$  is decreasing in  $\theta$  and

$$r_n(\Upsilon_n(\theta), \theta) \leq 2r_n(\infty, \theta).$$

Hence,  $\inf_{\gamma \in [0, \Upsilon_n(\theta)]} r_n(\gamma, \theta) \leq 2 \inf_{\gamma \geq 0} r(\gamma, \theta)$ . Some algebra shows that  $|\partial r_n(\gamma, \theta)/\partial \gamma| \leq A_n(\theta)$  for all  $\gamma$  and  $\theta$ . Therefore, for each  $j$ ,  $r_n(\gamma_j(\theta), \theta) = r_n(j\delta_n(\theta) + \delta_n(\theta), \theta) \geq r_n(j\delta_n(\theta), \theta) - \delta_n(\theta)A_n(\theta) \geq r_n(\gamma_j(\theta), \theta)/2$ . Let  $h_n = h(\gamma, \theta)$ . By Theorem 12,  $R^M(p, \widehat{p}_{h_n}) = O((\log n/n)^{\theta(\gamma+1)/(2\theta+d(\gamma+1))})$ . Let  $h_* \in \mathcal{H}_n$  minimize  $R^M(p, \widehat{p}_h)$  for  $h \in \mathcal{H}_n$ . Then  $R^M(p, \widehat{p}_{h_*}) \leq 2R^M(p, \widehat{p}_{h_n})$ . So,

$$\begin{aligned} R^M(p, \widehat{p}_{\widehat{h}}) &\leq d(\delta, \kappa) \frac{1 + \log 2}{n} + R^M(p, \widehat{p}_{h_*}) \\ &\leq d(\delta, \kappa) \frac{1 + \log 2}{n} + 2R^M(p, \widehat{p}_{h_n}) \\ &= d(\delta, \kappa) \frac{1 + \log 2}{n} + 2r_n(\gamma, \theta) \\ &= O\left(\frac{\log n}{n}\right)^{\theta(\gamma+1)/(2\theta+d(\gamma+1))}. \end{aligned}$$

□

**PROOF OF THEOREM 16.** (1) When  $h = 0$ ,  $\{\widehat{p}_h > \lambda\} = X$  and  $\{\widehat{q}_h > \lambda\} = Y$  so that  $\{\widehat{p}_h > \lambda\} \Delta \{\widehat{q}_h > \lambda\} = (X, Y)$ . Since  $P$  has a Lebesgue density, with probability one,  $d\widehat{P}_Z$  puts no mass on  $(X, Y)$  and, therefore,  $\Xi(0) = 0$ . By compactness

of  $S$ , if  $h \geq \text{diam}(S)$ , then  $\|\widehat{p}_h\|_\infty = \|\widehat{q}_h\|_\infty = \frac{1}{h^d v_d}$ , with the supremum attained by any  $z \in S$ . Thus, as  $h \rightarrow \infty$ ,  $\|\widehat{p}_h - \widehat{q}_h\|_\infty \rightarrow 0$  and consequently,  $\Xi(\infty) \rightarrow 0$ .

(2) Note that

$$\begin{aligned} \Xi(h) &= \rho(\widehat{p}_h, \widehat{q}_h, \widehat{P}_Z) = \int_{\{\widehat{p}_h \geq \lambda\} \Delta \{\widehat{q}_h \geq \lambda\}} d\widehat{P}_Z(z) \\ &= \int I(\widehat{p}_h(z) \geq \lambda, \widehat{q}_h(z) \leq \lambda) d\widehat{P}_Z(z) \\ &\quad + \int I(\widehat{p}_h(z) \leq \lambda, \widehat{q}_h(z) \geq \lambda) d\widehat{P}_Z(z). \end{aligned}$$

Define  $\xi(h) = \mathbb{E}(\Xi(h)|X, Y)$ . Then

$$\begin{aligned} \xi(h) &= \rho(\widehat{p}_h, \widehat{q}_h, P) \\ &= \int I(\widehat{p}_h(z) \geq \lambda, \widehat{q}_h(z) \leq \lambda) dP(z) \\ &\quad + \int I(\widehat{p}_h(z) \leq \lambda, \widehat{q}_h(z) \geq \lambda) dP(z) \\ &\stackrel{d}{=} 2 \int I(\widehat{p}_h(z) \geq \lambda, \widehat{q}_h(z) \leq \lambda) dP(z), \end{aligned}$$

where  $\stackrel{d}{=}$  denotes identity in distribution. Let  $\pi_h(z) = \mathbb{P}(\widehat{p}_h(z) \leq \lambda) = \mathbb{P}(\widehat{q}_h(z) \leq \lambda)$ . By Fubini's theorem and independence,

$$\begin{aligned} \mathbb{E}(\Xi(h)) &= \mathbb{E}(\xi(h)) \\ (35) \quad &= 2 \int_{\mathbb{R}^d} \mathbb{P}(\widehat{p}_h(z) \geq \lambda, \widehat{q}_h(z) \leq \lambda) dP(z) \\ &= 2 \int_{\mathbb{R}^d} \mathbb{P}(\widehat{p}_h(z) \geq \lambda) \mathbb{P}(\widehat{q}_h(z) \leq \lambda) dP(z) \\ &= 2 \int_{\mathbb{R}^d} \pi_h(z)(1 - \pi_h(z)) dP(z). \end{aligned}$$

Since  $\pi_h(z)(1 - \pi_h(z)) \leq 1/4$  for all  $n, h$  and  $z$ , (2) follows.

(3) Let  $W = (X, Y)$  be the  $2n$ -dimensional vector obtained by concatenating  $X$  and  $Y$  and define the event

$$\mathcal{A}_h = \{B(W_i, h) \cap B(W_j, h) = \emptyset, \forall i \neq j\}.$$

Let  $h$  be small enough such that  $\lambda n h^d v_d < 1$  (trivially satisfied if  $\lambda = 0$ ). Then, for any realization  $w$  of the vector  $W$  for which the event  $\mathcal{A}_h$  occurs,

$$\int I(\widehat{p}_h(z) \geq \lambda, \widehat{q}_h(z) \leq \lambda) dP(z) = \sum_{i=1}^{2n} P(B(w_i, h)).$$

By our assumptions,

$$2n\delta h^d v_d \leq \sum_{i=1}^{2n} P(B(w_i, h)) \leq 2n\bar{\Delta}h^d v_d.$$

Using the union bound, we also have

$$\mathbb{P}(\mathcal{A}_h^c) \leq \binom{2n}{2} (2h)^d v_d \bar{\Delta}.$$

Thus, it follows that, for fixed  $n$ ,  $\mathbb{E}(\xi(h)) \rightarrow 0$  as  $h \rightarrow 0$  according to

$$2n\delta h^d v_d \leq \mathbb{E}(\xi(h)) \leq h^d v_d 2\bar{\Delta} \max\{2^d n(2n - 1), 2n\}.$$

(4) By the same arguments used in the proof of point (1), for all  $h \geq h_*$ ,  $\xi(h) = 0$  almost everywhere with respect to the joint distribution of  $X$  and  $Y$ , and, therefore,  $\mathbb{E}(\xi(h)) = 0$ . Thus, we need only to consider the case  $0 < h \leq h_*$ .

Set  $p_{z,h} = P(B(z, h))$  and denote with  $X_{z,h}$  a random variable with distribution  $\text{Bin}(n, p_{z,h})$ . Then

$$\mathbb{P}(\hat{p}_h(z) = 0) = \mathbb{P}(X_{z,h} = 0) = (1 - p_{z,h})^n.$$

For each  $z \in S$ , set  $D(z, h) = \{z' \in S : \|z - z'\| < h\}$  and  $S_h = \{z : D(z, h) \neq S\}$ . Furthermore, set  $p_{h,\max} = \sup_{z \in S_h} \{p_{z,h}\}$  and  $p_{h,\min} = \inf_{z \in S_h} \{p_{z,h}\}$ . Then the expected instability can be written as

$$\mathbb{E}(\Xi(h)) = 2 \int_{S_h} \pi_h(z)(1 - \pi_h(z)) dP(z)$$

so that  $A_{h,n} \leq \mathbb{E}(\Xi(h)) \leq B_{h,n}$ , where

$$\begin{aligned} A_{h,n} &\equiv 2P(S_h)(1 - p_{h,\max})^n(1 - (1 - p_{h,\min})^n), \\ B_{h,n} &\equiv 2P(S_h)(1 - p_{h,\min})^n(1 - (1 - p_{h,\max})^n). \end{aligned}$$

We will now upper bound  $B_{h,n}/2$ . For the first term, we proceed as follows. There exists a sphere  $E = B(z_0, h_*/2)$  such that  $S \subset E$ . [E.g., choose any two points  $z, z'$  such that  $\|z - z'\| = h_*$ . Set  $z_0 = (z + z')/2$ .] Let  $A = B(z_0, h_*/2) - B(z_0, (h_* - h)/2)$ . We claim that  $S_h \subset A$ . This follows since if  $z \in A^c \cap S$  then  $z \in B(z_0, h/2)$  and then  $\sup_{z' \in S} \|z - z'\| \leq \sup_{z \in B(z_0, h/2), z' \in B(z_0, h_*/2)} \|z - z'\| = h$ . Thus, if  $z \in S_h$  then  $z \in A \cap S \subset A$ . Hence,

$$P(S_h) \leq P(A) \leq \bar{\Delta}\mu(A) = \bar{\Delta} \frac{((h_*/2)^d - (h/2)^d)\pi^{d/2}}{\Gamma((d/2) + 1)} \leq D_1(h_* - h),$$

where

$$D_1 = \frac{\pi^{d/2}h_*^{d-1}}{2^d\Gamma((d/2) + 1)}.$$

For the second term, let  $z_0 = \arg \min_z p_{z,h}$ . Then

$$\begin{aligned} 1 - p_{h,\min} &= 1 - P(B(z_0, h)) = P(B(z, h_*) - B(z_0, h)) \\ &= P(B(z, h_*) - B(z_0, h)) \leq \overline{\Delta}\mu(B(z, h_*) - B(z_0, h)) \\ &\leq \overline{\Delta} \frac{(h_*^d - h^d)\pi^{d/2}}{\Gamma((d/2) + 1)} = D_2(h_* - h), \end{aligned}$$

where  $D_2 = \frac{\pi^{d/2}h_*^{d-1}}{\Gamma((d/2)+1)}$ . The third term is bounded above by 1. Hence,  $B_n \leq D_1 D_2^n (h_* - h)^{n+1}$ .

Now we lower bound  $A_{h,n}/2$ . First, we claim that  $S_h$  contains the intersection of a sphere of radius  $r/2$  where  $r = h_* - h$ , with  $S$ . Indeed, let  $z \in S_h$ . Then there exists  $z' \in S$  such that  $\|z - z'\| \leq h_* = h + r$ . Let  $w \in B(z', r/2)$ . By the triangle inequality,  $\|w - z\| \geq h + r/2$ . So  $B(z', r/2) \cap S \subset S_h$ . Therefore,

$$\begin{aligned} P(S_h) &\geq P(B(z', r/2) \cap S) \geq \underline{\Delta}\mu(B(z', r/2) \cap S) \\ &\geq \delta \underline{\Delta}\mu(B(z', r/2)) = D_3(h_* - h)^d, \end{aligned}$$

where  $D_3 = \frac{\delta \underline{\Delta}\pi^{d/2}}{\Gamma((d/2)+1)}$ .

To lower bound the second term, Let  $z_0 = \arg \max_z p_{z,h}$ . Then

$$\begin{aligned} 1 - p_{h,\max} &= 1 - P(B(z_0, h)) = P(B(z, h_*) - B(z_0, h)) \\ &= P(B(z, h_*) - B(z_0, h)) \geq \underline{\Delta}\mu((B(z, h_*) - B(z_0, h)) \cap S) \\ &\geq \underline{\Delta}\delta \mu(B(z, h_*) - B(z_0, h)) = \underline{\Delta}\delta \frac{(h_* - h)^d \pi^{d/2}}{\Gamma(d/2 + 1)} \\ &= D_4(h_* - h)^d, \end{aligned}$$

where  $D_4 = \frac{\underline{\Delta}\delta \pi^{d/2}}{\Gamma(d/2+1)}$ . Thus,  $(1 - p_{h,\max})^n \geq D_4^n (h_* - h)^{nd}$ . For the third term, argue as above that  $1 - p_{h,\min} \leq D_2(h_* - h)$  so the third term is larger than  $1/2$  when  $h$  is close enough to  $h_*$ . Hence,  $A_n \geq \frac{D_3}{2} D_4^n (h_* - h)^{d(n+1)}$ .  $\square$

PROOF OF THEOREM 17. By our assumptions (see Section 2.1),

$$0 < \lim_{r \rightarrow 0} \frac{P(B(x, r))}{r^{d_i}} < \infty,$$

where  $d_i = \dim(S_i)$ , for any  $x$  outside of a set of  $P_i$  measure zero. By Theorem 5.7 in Mattila (1999),  $d_i$  is also the box-counting dimension of  $S_i$ . Thus,  $d^* = \max_i d_i$ . Combined with (29) this implies that, without loss of generality, we can assume that there exist constants  $\overline{C} > 0$  and  $\overline{\rho} > 0$  such that for every ball  $B$  of radius  $\rho < \overline{\rho}$  and center in  $L(\lambda)$ ,  $P(B) > \overline{C}\rho^{d^*}$ .

Let  $\mathcal{A}$  be a covering of  $L(\lambda)$  with balls of radius  $\rho/2$  and centers in  $L(\lambda)$ , with  $\rho < \overline{\rho}$ . By compactness of  $L$ ,  $|\mathcal{A}| \leq \overline{M}\rho^{-d^*}$ , where  $\overline{M}$  depends on  $d^*$  and  $L(\lambda)$  but not on  $\rho$ .

Next, by Lemma 2, on the event  $\mathcal{E}_{h,\varepsilon} = \{\|p_h - \widehat{p}_h\|_\infty < \varepsilon\}$ , the set  $\widehat{L}_h$  consists of  $k$  disjoint connected sets. Since  $\rho < \delta/2$ , this implies, on the same event, that  $\widehat{N}_h^G(\lambda) \geq k$ . Thus, on the event  $\mathcal{E}_{h,\varepsilon}$ , for some  $\varepsilon < \varepsilon_1$  to be specified below, a sufficient condition for the event  $\mathcal{O}_{h,n}$  to be verified is that every  $A \in \mathcal{A}$  contains at least one point from the set  $\widehat{J}_h \equiv \{i : \widehat{p}_h(X_i) \geq \lambda\}$  [similar arguments are used also in Cuevas, Febrero and Fraiman (2000), Biau, Cadre and Pellettier (2007)]. We conclude that the probability of  $\mathcal{O}_{h,n}^c$  is bounded from above by

$$\mathbb{P}(\mathcal{E}_{h,\varepsilon}^c) + \overline{M}\rho^{-d} \sup_{A \in \mathcal{A}_h} \mathbb{P}(\{X_i \notin A, \forall i \in \widehat{J}_h\} \cap \mathcal{E}_{h,\varepsilon}).$$

Since, on the event  $\mathcal{E}_{h,\varepsilon}$  the set  $J_{h_n} = \{i : p_{h_n}(X_i) \geq \lambda + \varepsilon\}$  is contained in  $\widehat{J}_h$ , we further have that, for each  $A \in \mathcal{A}_h$ ,

$$(36) \quad \mathbb{P}(\{X_i \notin A, \forall i \in \widehat{J}_h\} \cap \mathcal{E}_{h,\varepsilon}) \leq (1 - P(A \cap \{p_h \geq \lambda + \varepsilon\}))^n,$$

where the inequality stems from the identity among events

$$\{X_i \notin A, \forall i \in J_h\} = \bigcap_i \{ \{p_{h_n}(X_i) \geq \lambda + \varepsilon\} \cap A^c \cup \{p_{h_n}(X_i) < \lambda + \varepsilon\} \},$$

and the independence of the  $X_i$ 's. By Lemma 19, for any fixed  $0 < \tau < 1/2$ , there exists a point  $y \in L(\lambda) \cap L_h(\lambda + \varepsilon)$  such that  $B(y, \frac{\tau\rho}{2}) \subset A \cap L_h(\lambda + \varepsilon)$ , for all  $\varepsilon < \varepsilon(\rho, \tau)$ . Thus,

$$P(A \cap L_h(\lambda + \varepsilon)) \geq P\left(B\left(y, \frac{\tau\rho}{2}\right)\right) \geq \overline{C}\left(\frac{\tau\rho}{2}\right)^{d^*}$$

for all  $\varepsilon < \varepsilon(\rho, \tau)$ , where the second inequality is verified since  $\frac{\rho\tau}{2} < \overline{\rho}$ . Set  $\varepsilon(\rho) = \min\{\varepsilon_1, \varepsilon(\rho, \tau)\}$ . The result now follows from collecting all the terms and the inequality  $(1 - x)^n \leq e^{-nx}$ , valid for all  $0 \leq x \leq 1$ .  $\square$

**PROOF OF THEOREM 18.** Let  $\mathcal{A}_h$  be a covering of  $L_h(\lambda)$  by balls of radius  $\rho/2$  and centers in  $L_h(\lambda)$ . By the same arguments used in the proof of the Theorem 17, the probability of the event  $(\mathcal{O}_{h,n}^*)^c$  is bounded by

$$\mathbb{P}(\mathcal{E}_{h,\varepsilon}^c) + \overline{M}\rho^{-d} \sup_{A \in \mathcal{A}_h} \mathbb{P}(\{X_j^* \notin A, \forall j\} \cap \mathcal{E}_{h,\varepsilon}),$$

where the probability is over the original sample  $X = (X_1, \dots, X_n)$  and the bootstrap sample  $X^* = (X_1^*, \dots, X_n^*)$ . Here, the value of  $\varepsilon < \varepsilon_1$  used in the definition of the event  $\mathcal{E}_{h,\varepsilon}$  is to be specified below. Because of compactness of the support of  $P$ ,  $\overline{M}$  is a constant depending only  $d$  and  $S + B(0, \overline{h})$ .

For a set  $S \subseteq \mathbb{R}^d$ , we denote with  $S^{\otimes n}$  the  $n$ -fold Cartesian product of  $S$  and with  $P_{X^*|X=x}^h$  the conditional distribution of the bootstrap sample  $X^*$  given  $X = x$ , with  $x = (x_1, \dots, x_n)$ . Let  $\mathcal{E}_n = \{x \in S^{\otimes n} : \|p_h - \widehat{p}_h\|_\infty \leq \varepsilon\}$ , where  $\widehat{p}_h$  is the kernel density estimate based on  $x$ . Then, for each  $A \in \mathcal{A}_h$ ,

$$\mathbb{P}(\{X_j^* \notin A, \forall j\} \cap \mathcal{E}_{h,\varepsilon}) = E_X(P_{X^*|X}((A^c)^{\otimes n}); \mathcal{E}_n),$$

where, if  $X \sim P$ ,  $E_X(f(X); \mathcal{E}) \equiv \int_{\{x \in \mathcal{E}\}} f(x) dP(x)$ . For every  $x \in \mathcal{E}_n$ , by the conditional independence of  $X^*$  given  $X = x$ ,

$$\begin{aligned} P_{X^*|X=x}((A^c)^{\otimes n}) &= \left(1 - \frac{\int_{A \cap L_h(\lambda)} \widehat{p}_h(v) dv}{\int_{\{\widehat{p}_h \geq \lambda\}} \widehat{p}_h(v) dv}\right)^N \\ &\leq \left(1 - \frac{\int_{A \cap L_h(\lambda+\varepsilon)} (p_h - \varepsilon) d\mu}{V(h, \varepsilon)}\right)^N, \end{aligned}$$

where

$$V(h, \varepsilon) = \int_{L_h(\max\{\lambda-\varepsilon, 0\})} (p_h + \varepsilon) d\mu.$$

By Lemma 19, for any fixed  $\tau < 1/2$  and each  $h$ , there exists a point  $y \in L_h(\lambda) \cap L_h(\lambda + \varepsilon)$  such that  $B(y, \frac{\tau\rho}{2}) \subset A \cap L_h(\lambda + \varepsilon)$ , for all  $\varepsilon < \varepsilon(\rho, \tau)$ . Thus,

$$\begin{aligned} \int_{A \cap L_h(\lambda+\varepsilon)} (p_h - \varepsilon) d\mu &\geq \int_{B(y, \tau\rho/2)} (p_h - \varepsilon) d\mu \\ &= \int_{B(y, \tau\rho/2)} p_h d\mu - \varepsilon\mu\left(B\left(y, \frac{\tau\rho}{2}\right)\right). \end{aligned}$$

Next,

$$V(h, \varepsilon) = \int_{L_h(\lambda)} p_h d\mu + \varepsilon\mu(L_h(\max\{\lambda - \varepsilon, 0\})) + \int_{L_h(\lambda) - L_h(\max\{\lambda-\varepsilon, 0\})} p_h d\mu.$$

Following the proof of Lemma 19, one can verify that, because of assumption (G),  $\inf_{h \in (0, \bar{h})} \mu(L_h(\lambda) - L_h(\max\{\lambda - \varepsilon, 0\})) \rightarrow 0$ , as  $\varepsilon \rightarrow 0$ . Thus,

$$\frac{\int_{A \cap L_h(\lambda+\varepsilon)} (p_h - \varepsilon) d\mu}{V(h, \varepsilon)} \geq \frac{\int_{B(y, \tau\rho/2)} p_h d\mu}{\int_{L_h(\lambda)} p_h d\mu} (1 + o(1))$$

as  $\varepsilon \rightarrow 0$ . Then using (30) and the facts  $\tau < 1/2$  and  $\int_{L_h(\lambda)} p_h d\mu \leq 1$  for each  $h$ , we conclude that there exists a  $\varepsilon(\rho, \tau)$  such that

$$\frac{\int_{A \cap L_h(\lambda+\varepsilon)} (p_h - \varepsilon) d\mu}{V(h, \varepsilon)} \geq C\rho^d$$

for all  $0 < \varepsilon < \varepsilon(\rho, \tau)$  and for some appropriate constant  $C$ , independent of  $\rho$  and  $h$ . Thus,

$$P_{X^*|X=x}((A^c)^{\otimes n}) \leq e^{-NC\rho^d}$$

and the results now follows by setting  $\varepsilon(\rho) = \min\{\varepsilon_1, \varepsilon(\rho, \tau)\}$ .  $\square$

LEMMA 19. Assume conditions (C2) and (G). Then, for any  $0 < \tau < 1$  and  $\rho > 0$ , there exists a positive number  $\varepsilon(\rho, \tau)$  such that, for all  $\varepsilon < \varepsilon(\rho, \tau)$ ,

$$(37) \quad \sup_{h \in (0, \bar{h})} \sup_{x \in L(\lambda)} \text{dist}(x, L_h(\lambda + \varepsilon)) < \tau\rho.$$



PROOF. The claim follows by minor modifications of the arguments used in the Appendix of [Biau, Cadre and Pellettier \(2007\)](#). We provide some details for completeness and refer to [Lee \(2003\)](#) for background. Because of assumption (G) and in virtue of the regular level set theorem [see, e.g., [Lee \(2003\)](#), Corollary 8.10], for any  $\varepsilon \in (0, \varepsilon_1)$  and  $h \in (0, \bar{h})$ , the set  $\{x : p_h(x) = \lambda + \varepsilon\}$  is a closed embedded submanifold of  $\mathbb{R}^d$ . Let  $r(\varepsilon, h)$  be the maximal radius of the tubular neighborhood around  $\{x : p_h(x) = \lambda + \varepsilon\}$ . Set  $\bar{r}_h = \inf_{\varepsilon < \varepsilon_1} r(\varepsilon, h)$  and notice that  $\bar{r}_h > 0$  is positive for each  $h \in (0, \bar{h})$ . Then, following the proof of [Biau, Cadre and Pellettier \[\(2007\), Proposition A.2\]](#) if  $\varepsilon < \varepsilon_1$ , for any  $h \in (0, \bar{h})$ ,

$$(38) \quad \sup_{x \in \partial L_h(\lambda)} \text{dist}(x, L_h(\lambda + \varepsilon)) \leq C_g^{-1} \varepsilon,$$

where  $C_g$  in the same constant appearing in (28) [see equation (A.1) in [Biau, Cadre and Pellettier \(2007\)](#)]. In fact, since  $C_g$  does not depend on  $h$ , (38) holds uniformly over  $h \in (0, \bar{h})$ . Set  $\varepsilon(\rho, \tau) = \sup\{\varepsilon \in (0, \varepsilon_1) : C\varepsilon < \tau\rho\}$ . Then as  $L(\lambda) \subseteq L_h(\lambda)$  by (C2)(b), (37) is verified for each  $\varepsilon < \varepsilon(\rho, \tau)$ .  $\square$

### APPENDIX: THE GEOMETRIC DENSITY

In this section, we describe in detail our assumptions on the unknown distribution  $P$ . For the sake of completeness, we provide the basic definitions of Hausdorff measure, Hausdorff dimension, and rectifiability. We refer the reader to [Evans and Gariepy \(1992\)](#), [Mattila \(1999\)](#), [Ambrosio, Fusco and Pallara \(2000\)](#) and [Federer \(1969\)](#) for all the relevant geometric and measure theoretic background.

Let  $k \in [0, \infty)$ . The  $k$ -dimensional Hausdorff measure of a set  $E$  in  $\mathbb{R}^d$  is defined as  $\mathcal{H}^k(E) \equiv \lim_{\delta \downarrow 0} \mathcal{H}_\delta^k(E)$ , where, for  $\delta \in (0, \infty]$ ,

$$\mathcal{H}_\delta^k(E) = \frac{v_k}{2^k} \inf \left\{ \sum_{i \in I} (\text{diam}(E_i))^k : \text{diam}(E_i) < \delta \right\},$$

where the infimum is over all the countable covers  $\{E_i\}_{i \in I}$  of  $E$ , with the convention  $\text{diam}(\emptyset) = 0$ . The Hausdorff dimension of a set  $E \subset \mathbb{R}^d$  is

$$\inf\{k \geq 0 : \mathcal{H}^k(E) = 0\}.$$

Note that  $\mathcal{H}^0$  is the counting measure, while  $\mathcal{H}^d$  coincides with the (outer) Lebesgue measure. If  $k < d$ , we will refer to any  $\mathcal{H}^k$ -measureable set as a set of lower-dimension. When  $1 \leq k < d$  is an integer,  $\mathcal{H}^k(E)$  coincides with the  $k$ -dimensional area of  $E$ , if  $E$  is contained in a  $\mathcal{C}^1$   $k$ -dimensional manifold embedded in  $\mathbb{R}^d$ .

The set  $E$  is said to be  $\mathcal{H}^k$ -rectifiable if  $k$  is an integer,  $\mathcal{H}^k(E) < \infty$  and there exist countably many Lipschitz functions  $f_i : \mathbb{R}^k \mapsto \mathbb{R}^d$  such that

$$\mathcal{H}^k \left( E - \bigcup_{i=0}^{\infty} f_i(\mathbb{R}^k) \right).$$

A Radon measure  $\nu$  in  $\mathbb{R}^d$  is said to be  $k$ -rectifiable if there exists a  $\mathcal{H}^k$ -rectifiable set  $S$  and a Borel function  $f : S \mapsto \mathbb{R}^d$  such that

$$\nu(A) = \int_{A \cap S} f(x) d\mathcal{H}^k(x)$$

for each measurable set  $A \subseteq \mathbb{R}^d$ .

Throughout this article, we assume that  $P$  is a finite mixture of probability measures supported on disjoint compact sets of possibly different integral Hausdorff dimensions. Formally, for each Borel set  $A \subseteq \mathbb{R}^d$  and for some integer  $m$ ,

$$P(A) = \sum_{i=1}^m \pi_i P_i(A),$$

where  $\pi$  is a point in the interior of the  $(m - 1)$ -dimensional standard simplex and each  $P_i$  is a  $d_i$ -rectifiable Radon measure with compact and connected support  $S_i$ , where  $d_i \in \{0, 1, \dots, d\}$  and  $S_i \cap S_j = \emptyset$ , for each  $i \neq j$ . Notice that we also have  $\max_i \mathcal{H}^{d_i}(S_i) < \infty$ . By Theorem 3.2.18 in Federer (1969), each of the lower-dimensional rectifiable sets comprising the support of  $P$ , can be represented as the union of  $\mathcal{C}^1$  embedded submanifolds, almost everywhere  $P$ . Thus, we are essentially allowing  $P$  to be a mixture of distributions supported on disjoint submanifolds of different dimensions and finite sets.

Our assumptions imply that, for every mixture component  $P_i$ , there exists a  $\mathcal{H}^{d_i}$ -measurable real valued function  $p_i$  such that such that

$$(39) \quad p_i(x) = \begin{cases} \lim_{h \rightarrow 0} \frac{P_i(B(x, h))}{v_{d_i} h^{d_i}} > 0, & \text{if } x \in S_i, \\ 0, & \text{if } x \notin S_i, \end{cases}$$

where  $v_{d_i}$  is the volume of the unit Euclidean ball in  $\mathbb{R}^{d_i}$ . See, for instance, Mattila [(1999), Corollary 17.9] or Ambrosio, Fusco and Pallara [(2000), Theorem 2.83]. Indeed,  $p_i$  is a density function with respect to  $\mathcal{H}^{d_i}$  since, for any measurable set  $A$ ,

$$P_i(A) = \int_{A \cap S_i} p_i(x) d\mathcal{H}^{d_i}(x),$$

where  $\mathcal{H}^{d_i}$  denotes the  $d_i$ -dimensional Hausdorff measure on  $\mathbb{R}^d$ .

We do not assume any knowledge of the probability measures comprising the mixture  $P$ , of their number, supports and dimensions, nor of the vector of mixing probabilities  $\pi$ .

Recall that the geometric density is the extended real-valued function defined as

$$p(x) = \lim_{h \downarrow 0} \frac{P(B(x, h))}{v_d h^d}, \quad x \in \mathbb{R}^d.$$

Below, we list the key properties of the geometric density. Notice, in particular, that  $p$  is not a probability density with respect to  $\mu$ , since, in general,  $0 \leq \int_{\mathbb{R}^d} p(x) d\mu(x) \leq 1$ .

PROPOSITION 20. *The geometric density satisfies the following properties:*

- (i)  $p(x) = \infty$  if and only if  $x \in S_i$  with  $\dim(S_i) < d$ , almost everywhere  $P$ ,
- (ii)  $p(x) = \pi_i p_i(x) < \infty$  if and only if  $x \in S_i$  with  $\dim(S_i) = d$ , almost everywhere  $\mu$ ,
- (iii)  $\mu(\{x : p(x) = \infty\}) = 0$ ,
- (iv) if  $x \notin S$ , then  $p(x) = 0$ ,
- (v)  $S = \{x : p(x) > 0\}$ .

PROOF. If  $S_i$  has dimension  $d$ , then, by the Lebesgue theorem,

$$p(x) = \lim_{h \downarrow 0} \frac{P(B(x, h))}{v_d h^d} = \pi_i p_i(x) < \infty,$$

$\mu$ -almost everywhere on  $S_i$ . Similarly, if  $d_i < d$ , then, by (39),

$$p(x) = \lim_{h \downarrow 0} \frac{P(B(x, h))}{v_d h^d} = \lim_{h \downarrow 0} \frac{v_{d_i} h^{d_i} P_i(B(x, h))}{v_d h^d} = \infty,$$

since  $\frac{v_{d_i} h^{d_i}}{v_d h^d} \rightarrow \infty$  as  $h \downarrow 0$ ,  $\mathcal{H}^{d_i}$ -almost everywhere on  $S_i$ . Thus, part (i) and (ii) follow. Part (iii) is a direct consequence of (i) and (ii), while parts (iv) and (v) stem directly from the definition of support.  $\square$

As a final remark, even though the geometric density  $p$  is very different from the mixture densities  $p_i$ , for our clustering purposes, we need only to concern ourselves with estimating the level sets of  $p$ .

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