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# Fast rates for plug-in estimators of density level sets

PHILIPPE RIGOLLET <sup>\*</sup> and RÉGIS VERT <sup>†</sup>

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## Abstract

In the context of density level set estimation, we recall the notion of  $\gamma$ -exponent of a density at a certain level. This notion is similar to Tsybakov's margin assumption and allows us to prove fast rates of convergence for general plug-in methods, up to order  $n^{-1}$  when the density is supposed to be smooth in a neighborhood of the level under consideration. Lower bounds proving optimality of the rates in a minimax sense are also provided.

**Mathematics Subject Classifications:** Primary 62G05, Secondary 62C20, 62G05, 62G20.

**Key Words:** Density level set, plug-in estimators, fast rates of convergence, minimax lower bounds.

**Short title:** Plug-in density level set estimation.

## 1 Introduction

Let  $Q$  be a positive  $\sigma$ -finite measure on  $\mathcal{X} \subseteq \mathbb{R}^d$ . Consider i.i.d random vectors  $(X_1, \dots, X_n)$  with distribution  $P$ , having an unknown probability density  $p$  with respect to the measure  $Q$ . For a fixed  $\lambda > 0$ , we are interested in the estimation of the  $\lambda$ -level set of the density  $p$ :

$$\Gamma_p(\lambda) \triangleq \{x \in \mathcal{X} : p(x) \geq \lambda\} .$$

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Throughout the paper we fix  $\lambda > 0$  and when no confusion is possible we use the notation  $\Gamma(\lambda)$  or simply  $\Gamma$  instead of  $\Gamma_p(\lambda)$ . When  $Q$  is the Lebesgue measure on  $\mathbb{R}^d$ , density level sets typically correspond to minimum volume sets of given  $P$ -probability mass, as shown in Polonik (1997). More generally, if  $Q$  is an arbitrary probability distribution on  $\mathbb{R}^d$ , density level sets correspond to the critical regions of likelihood ratio (Neyman-Pearson) tests, which are known to be optimal for testing the hypothesis  $P$  versus the alternative  $Q$ .

Here are two possible applications of density level set estimation.

**Anomaly detection:** the goal is to detect an abnormal observation from a sample (see Schölkopf et al., 2001). One way to deal with that problem is to assume that abnormal observations do not belong to a group of concentrated observations. In this framework, observations are considered as abnormal when they do not belong to  $\Gamma(\lambda)$  for some fixed  $\lambda \geq 0$ . The special case  $\lambda = 0$ , which corresponds to support estimation has been examined by Devroye and Wise (1980). In the general case,  $\lambda$  can be considered as a tolerance level for anomalies: the smaller  $\lambda$ , the fewer observations are considered as being abnormal. In particular, it is often the case that the user has a fixed budget, allowing him to qualify only a limited fraction of the data as outliers.

**Unsupervised or semi-supervised classification:** these two problems amount to identify areas where the observations are concentrated with possible use of some available labels for the semi-supervised case. More precisely it can be assumed that the connected components of  $\Gamma(\lambda)$ , for a fixed  $\lambda$ , are clusters of homogeneous observations as described in Hartigan (1975). Again, the bigger the  $\lambda$ , the smaller the clusters.

**Remark 1.1** *In both applications, the choice of  $\lambda$  can be left to the user depending on its tolerance to anomalies or the desired number of clusters.*

There are essentially two approaches towards estimating density level sets from the sample  $(X_1, \dots, X_n)$ : *plug-in* methods where the density  $p$  in the expression for  $\Gamma_p(\lambda)$  is replaced by its estimate computed from the sample, and *direct* methods which are based on empirical excess-mass maximization (see Hartigan, 1987; Müller and Sawitzki, 1987).

While local versions of direct methods have been deeply analyzed and proved to be optimal in a minimax sense, over a certain family of well-behaved distributions (see Tsybakov, 1997), and although reasonable implementations have been recently proposed (see for instance Steinwart et al.,

2005), they are still not very easy to use for practical purposes, compared to plug-in methods. Indeed, it is common to estimate density level sets for different level values -typically when the goal is to compute a density level set of pre-specified probability mass (or acceptance rate) and unknown density level. In that case, using direct methods, one has to run an optimization procedure several times, one for different density level values, then choose a posteriori the most suited level according to the desired rejection rate. Plug-in methods do not involve such a complex process: the density estimation step is only performed once and the construction of a density level set estimate simply amounts to thresholding the density estimate at the desired level.

On the other hand, in the related context of binary classification where more theoretical advances have been developed, the different analyses proposed so far have mainly supported a belief in the superiority of direct methods. Yang (1999) shows that, under general assumptions, plug-in rules cannot achieve a classification error risk convergence rate faster than  $O(1/\sqrt{n})$  (where  $n$  is the size of the data sample), and suffer from the curse of dimensionality. On the contrary, under slightly different assumptions, direct methods achieve this rate  $O(1/\sqrt{n})$  whatever the dimensionality (see e.g. Vapnik, 1998; Devroye et al., 1996; Tsybakov, 2004b), and can even reach faster convergence rates- up to  $O(1/n)$ - under *Tsybakov's margin assumption* (see Mammen and Tsybakov, 1999; Tsybakov, 2004b; Tsybakov and van de Geer, 2005; Tarigan and van de Geer, 2006). This contributed to raising some pessimism concerning plug-in methods. Nevertheless such a comparison between plug-in methods and direct methods is far from being legitimate, since the aforementioned analyzes of both plug-in methods and direct ones have been carried out under the different sets of assumptions (those sets are not disjoint, but none of them is included in the other).

Recently, Audibert and Tsybakov (2005) have introduced a new type of assumption dealing with the smoothness of the *regression function* in the standard classification framework, under which they derive fast convergence rates- even faster than  $O(1/n)$  in some situations- for plug-in classification rules based on local polynomial estimators. This new result reveals that plug-in methods should not be considered as inferior to direct methods and, more importantly, that this new type of assumption on the regression function is a critical point in the general analysis of classification procedures.

In this paper we extend such positive results to the density level set estimation (DLSE) framework: we revisit the analysis of plug-in density level set estimators, and show that they can be also very efficient under smoothness assumptions on the underlying density function  $p$ . Related papers are

Baíllo et al. (2001) and Baíllo (2003), who investigate plug-in rules based on a certain type of kernel density estimates. Baíllo (2003) derives almost sure rates of convergence for a quantity different from the one studied here. It is interesting to observe that she introduces a condition similar to the  $\gamma$ -exponent used here. The particular case  $\lambda = 0$ , corresponds to estimation of the support of density  $p$  and is often applied to anomaly detection. Following the pioneer paper of Devroye and Wise (1980), this problem has received more attention than the general case  $\lambda \geq 0$  and has been treated using plug-in methods for example by Cuevas and Fraiman (1997). Unlike the previously cited papers, we derive fast rates of convergence and prove that these rates are optimal in a minimax sense.

A general plug-in approach has been studied previously by Molchanov (1998), where a result on the asymptotic distribution of the Hausdorff distance is given. In a recent paper, Cuevas et al. (2006) study general plug-in estimators of the level sets. Under very general assumptions they derive consistency with respect to the Hausdorff metric and the measure of the symmetric difference. However, this very general framework does not allow them to derive rates of convergence.

This paper is organized as follows. Section 2 introduces the notation and definitions. Section 3 presents the main result, that is a new bound on the error of penalized plug-in estimators based on general density estimators that satisfy a certain exponential inequality. As an example we prove that kernel density estimators are valid for this method. The upper bounds are proved to be optimal in Section 4, where we prove the corresponding minimax lower bounds.

## 2 Notation and Setup

For any vector  $x \in \mathbb{R}^d$ , denote by  $x^{(j)}$  its  $j$ th coordinate,  $j = 1, \dots, d$ . Denote by  $\mathcal{B}_\alpha(x, r)$  the closed ball in  $\mathcal{X}$  centered at  $x \in \mathcal{X}$  and of radius  $r > 0$  with respect to the norm  $\|\cdot\|_\alpha$ ,  $1 \leq \alpha \leq \infty$  defined by

$$\|x\|_\alpha \triangleq \left( \sum_{i=1}^d |x^{(i)}|^\alpha \right)^{1/\alpha}.$$

and

$$\|x\|_\infty \triangleq \max_{i=1, \dots, d} |x^{(i)}|.$$

The probability and expectation with respect to the joint distribution of  $(X_1, \dots, X_n)$  are denoted by  $\mathbb{P}$  and  $\mathbb{E}$  respectively. For any function

$f : \mathbb{R}^d \rightarrow \mathbb{R}$ , we denote by  $\|f\|_\infty = \sup_{x \in \mathbb{R}^d} |f(x)|$  the sup-norm of  $f$  and by  $\|f\| = (\int_{\mathbb{R}^d} f^2(x) dx)^{1/2}$  its  $L_2$ -norm. Throughout the paper, we denote by  $c_j$  positive constants and by  $A^c$  the complement of the set  $A$ .

## 2.1 Penalized plug-in rules

For a fixed  $\lambda > 0$ , the plug-in estimator of  $\Gamma(\lambda)$  is defined by

$$\hat{\Gamma}(\lambda) = \{x \in \mathcal{X} : \hat{p}_n(x) \geq \lambda\},$$

where  $\hat{p}_n$  is a nonparametric estimator of  $p$ . For example,  $\hat{p}_n$  can be a kernel density estimator of  $p$ ,

$$\hat{p}_n(x) = \hat{p}_{n,h}(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right), \quad x \in \mathcal{X},$$

where  $K : \mathbb{R}^d \rightarrow \mathbb{R}$  is a suitably chosen kernel and  $h > 0$  is the bandwidth parameter.

It is sometimes the case, for some applications that  $\hat{\Gamma}$  is required to be included in  $\Gamma$  with high probability (see, e.g., Rigollet, 2006). For this reason, we consider in this paper the more general family of *penalized plug-in rules*  $\tilde{\Gamma}_{\ell_n}$  defined as follows:

$$\tilde{\Gamma}_{\ell_n} = \tilde{\Gamma}_{\ell_n}(\lambda) = \hat{\Gamma}(\lambda + \ell_n) = \{x \in \mathcal{X} : \hat{p}_n(x) \geq \lambda + \ell_n\},$$

where  $(\ell_n)$  is a non-negative sequence that typically tends to 0 as  $n$  tends to infinity. This family includes in particular the estimator  $\hat{\Gamma}$  when  $\ell_n$  is taken equal to 0.

## 2.2 Measures of performance

Recall that  $Q$  is a positive  $\sigma$ -finite measure on  $\mathcal{X}$  and define the measure  $\tilde{Q}_\lambda$  that has density  $|p(\cdot) - \lambda|$  with respect to  $Q$ . To assess the performance of a density level set estimator, we use the two pseudo-distances between closed sets  $G_1$  and  $G_2 \subseteq \mathcal{X}$ :

- (i) The  $Q$ -measure of the symmetric difference between  $G_1$  and  $G_2$ :

$$d_\Delta(G_1, G_2) = Q(G_1 \Delta G_2).$$

- (ii) The  $\tilde{Q}_\lambda$ -measure of the symmetric difference between  $G_1$  and  $G_2$ :

$$d_H(G_1, G_2) = \tilde{Q}_\lambda(G_1 \Delta G_2) = \int_{G_1 \Delta G_2} |p(x) - \lambda| dQ(x).$$

The quantity  $d_\Delta(G_1, G_2)$  is a standard and natural way to measure the distance between two sets  $G_1$  and  $G_2$ . Another way to measure the quality of  $\hat{G}$  is to compute its *excess-mass*  $H(\hat{G})$  defined as follows (Hartigan, 1987; Müller and Sawitzki, 1987):

$$H(\hat{G}) = P(\hat{G}) - \lambda Q(\hat{G}) .$$

Excess-mass measures how the  $P$ -probability mass concentrates in the region  $\hat{G}$ , and it is maximized by  $\Gamma = \Gamma(\lambda)$ . Hence, it acts as a risk functional in the DLSE framework and it is natural to measure the performance of an estimator  $\hat{G}$  by its *excess-mass deficit*  $H(\Gamma) - H(\hat{G}) \geq 0$ . Further justifications for the well-foundedness of the excess mass criterion can be found in Polonik (1995). Note that for any measurable set  $G \subseteq \mathcal{X}$ , the excess-mass  $H(G)$  can be written

$$H(G) = \int_G (p(x) - \lambda) dQ(x) .$$

Thus, we can rewrite,

$$\begin{aligned} H(\Gamma) - H(\hat{G}) &= \int_{\mathcal{X}} (\mathbb{1}_{\{p(\cdot) \geq \lambda\}}(x) - \mathbb{1}_{\hat{G}}(x)) (p(x) - \lambda) dQ(x) \\ &= \int_{\Gamma \Delta \hat{G}} |p(x) - \lambda| dQ(x) = d_H(\hat{G}, \Gamma) . \end{aligned}$$

This explains the notation  $d_H$ . The next definition allows us to link  $d_H$  to  $d_\Delta$ .

**Definition 2.1** *For any  $\lambda, \gamma \geq 0$ , a function  $f : \mathcal{X} \rightarrow \mathbb{R}$  is said to have  $\gamma$ -exponent at level  $\lambda$  with respect to  $Q$  if there exist constants  $c_0 > 0$  and  $\varepsilon_0 > 0$  such that, for all  $0 < \varepsilon \leq \varepsilon_0$ ,*

$$Q \{x \in \mathcal{X} : |f(x) - \lambda| \leq \varepsilon\} \leq c_0 \varepsilon^\gamma .$$

This condition has been introduced in Polonik (1995). It is a generalization to any level  $\lambda > 0$  instead of  $1/2$ , of the celebrated margin assumption formulated in Mammen and Tsybakov (1999) and Tsybakov (2004a). The exponent  $\gamma$  controls the slope of the function around level  $\lambda$ . When  $\gamma = 0$ , the condition is loose and the density is allowed to have flat parts at level  $\lambda$ . When  $\gamma$  is positive, the function  $f$  has no flat part at level  $\lambda$ . A standard case corresponds to  $\gamma = 1$ , arising for instance in the case where the gradient of  $f$  has a coordinate bounded away from 0 in a neighborhood of  $\{f = \lambda\}$ . If  $\gamma < 1$ , we call  $\lambda$  a *critical level*. To illustrate such cases, assume that  $Q$  is the Lebesgue measure on  $\mathbb{R}^d$  denoted here by  $\text{Leb}_d$ . Let  $q$  be a positive number such that  $q > d$  and consider a function  $f$  on  $\mathbb{R}^d$  such that

- $f(x) = \lambda + \|x - x_0\|_2^q$ , for all  $x \in \mathbb{R}^d$  in a neighborhood of  $x_0$  and
- $f(x) \leq \lambda/2$  for any  $x \in \mathbb{R}^d$  outside of this neighborhood.

Then,  $\text{Leb}_d \{|f - \lambda| \leq \varepsilon\} = c_1 \varepsilon^{d/q}$ , for some constant  $c_1 > 0$  and for  $\varepsilon$  small enough.

We now show that the pseudo-distances  $d_\Delta$  and  $d_H$  are linked when the density  $p$  has  $\gamma$ -exponent at level  $\lambda$  with  $\gamma > 0$ . Remark first that when  $\|p\|_\infty \leq L_0 < \infty$ ,  $d_\Delta$  dominates  $d_H$  in the sense that for any  $G_1, G_2 \subseteq \mathcal{X}$ , we have

$$d_H(G_1, G_2) \leq \max(\lambda, L_0) d_\Delta(G_1, G_2).$$

This inequality is valid whatever  $\gamma \geq 0$ . When  $\gamma > 0$ , the following proposition holds.

**Proposition 2.1** *Fix  $\lambda > 0, \gamma > 0$  and  $L_Q > 0$ . The two following statements are equivalent.*

- (i)  $\exists c > 0$  and  $\varepsilon_0 > 0$ , such that for any  $0 < \varepsilon \leq \varepsilon_0$ , we have

$$Q \{x \in \mathcal{X} : |p(x) - \lambda| \leq \varepsilon\} \leq c\varepsilon^\gamma.$$

- (ii)  $\exists c' > 0$  and  $\varepsilon_1 > 0$ , such that for any  $0 < \varepsilon \leq \varepsilon_1$ , we have

$$Q \{x \in \mathcal{X} : |p(x) - \lambda| \leq \varepsilon\} \leq L_Q$$

and for all  $C \subseteq \mathcal{X}$  satisfying  $Q(C) \leq L_Q$ , we have

$$Q(C) \leq c' \left( \int_C |p(x) - \lambda| dQ(x) \right)^{\frac{\gamma}{1+\gamma}}. \quad (2.1)$$

In particular, taking  $C = G_1 \Delta G_2$  with  $G_1$  and  $G_2$  two closed subsets of  $\mathcal{X}$  such that  $Q(G_1) + Q(G_2) \leq L_Q$ , if the density  $p$  has  $\gamma$ -exponent at level  $\lambda$  w.r.t  $Q$ , we have

$$d_\Delta(G_1, G_2) \leq c' (d_H(G_1, G_2))^{\frac{\gamma}{1+\gamma}}.$$

PROOF. We first prove (i)  $\Rightarrow$  (ii). Define

$$\varepsilon_1 = \min \left[ \varepsilon_0, \left( \frac{L_Q}{c(1+\gamma)} \right)^{1/\gamma} \right].$$

Remark that for any  $0 < \varepsilon \leq \varepsilon_1$ , we have

$$Q \{x \in \mathcal{X} : |p(x) - \lambda| \leq \varepsilon\} \leq c\varepsilon^\gamma \leq c\varepsilon_1^\gamma = \frac{L_Q}{1+\gamma} \leq L_Q.$$



Define  $\mathcal{A}_\varepsilon = \{x : |p(x) - \lambda| > \varepsilon\}$ , for all  $0 < \varepsilon \leq \varepsilon_0$ . For any measurable set  $C \subset \mathcal{X}$ , we have

$$\begin{aligned} \int_C |p(x) - \lambda| dQ(x) &\geq \varepsilon Q(C \cap \mathcal{A}_\varepsilon) \\ &\geq \varepsilon [Q(C) - Q(\mathcal{A}_\varepsilon^c)] \\ &\geq \varepsilon [Q(C) - c\varepsilon^\gamma], \end{aligned}$$

where the last inequality is obtained using (i). Maximizing the last term w.r.t  $\varepsilon > 0$ , we get

$$\left( \int_C |p(x) - \lambda| dQ(x) \right)^{\frac{\gamma}{1+\gamma}} \geq Q(C) \left( \frac{\gamma}{1+\gamma} \right)^{\frac{\gamma}{1+\gamma}} \left( \frac{1}{1+\gamma} \right)^{\frac{1}{1+\gamma}} c^{-1/(1+\gamma)}.$$

This yields (2.1) with  $c' = e^{-2/e} c^{1/(1+\gamma)}$ . Note that the maximum is obtained for  $\varepsilon = \left( \frac{Q(C)}{c(1+\gamma)} \right)^{1/\gamma} \leq \varepsilon_0$  and (i) is valid for this particular  $\varepsilon$ .

We now prove that (ii)  $\Rightarrow$  (i). Consider  $\varepsilon_1 > 0$  such that  $Q(\mathcal{A}_\varepsilon^c) \leq L_Q$  for any  $0 < \varepsilon \leq \varepsilon_1$  and  $c' > 0$  such that (2.1) is satisfied for any  $C \subseteq \mathcal{X}$ ,  $Q(C) \leq L_Q$ . Taking  $C = \mathcal{A}_\varepsilon^c$  in (2.1) yields

$$\begin{aligned} Q\{x : |p(x) - \lambda| \leq \varepsilon\} &= Q(\mathcal{A}_\varepsilon^c) \\ &\leq c' \left( \int_{\mathcal{A}_\varepsilon^c} |p(x) - \lambda| dQ(x) \right)^{\frac{\gamma}{1+\gamma}} \\ &\leq c' (\varepsilon Q(\mathcal{A}_\varepsilon^c))^{\frac{\gamma}{1+\gamma}}. \end{aligned}$$

Therefore,

$$Q\{x : |p(x) - \lambda| \leq \varepsilon\} \leq (c')^{1+\gamma} \varepsilon^\gamma.$$

This inequality yields (i) with  $\varepsilon_0 = \varepsilon_1$  and  $c = (c')^{1+\gamma}$ . ■

### 2.3 Classes of densities

Fix  $\beta > 0$  and  $\lambda > 0$ . For any  $d$ -tuples  $s = (s_1, \dots, s_d) \in \mathbb{N}^d$  and  $x = (x_1, \dots, x_d) \in \mathcal{X}$ , we define  $|s| = s_1 + \dots + s_d$ ,  $s! = s_1! \dots s_d!$  and  $x^s = x_1^{s_1} \dots x_d^{s_d}$ . Let  $D^s$  denote the differential operator

$$D^s = \frac{\partial^{s_1 + \dots + s_d}}{\partial x_1^{s_1} \dots \partial x_d^{s_d}}.$$

Denote by  $\lfloor \beta \rfloor$  the maximal integer that is strictly smaller than  $\beta$  and fix  $x_0 \in \mathcal{X}$ . For any real valued function  $g$  on  $\mathcal{X}$  that is  $\lfloor \beta \rfloor$ -times continuously differentiable at point  $x_0$ , we denote by  $g_{x_0}^{(\beta)}$  its Taylor polynomial of degree  $\lfloor \beta \rfloor$  at point  $x_0$ :

$$g_{x_0}^{(\beta)}(x) = \sum_{|s| \leq \lfloor \beta \rfloor} \frac{(x - x_0)^s}{s!} D^s g(x_0).$$

Let  $L > 0$  and denote by  $\Sigma(\beta, L, x_0)$  the set of functions  $g : \mathcal{X} \rightarrow \mathbb{R}$  that are  $\lfloor \beta \rfloor$ -times continuously differentiable at point  $x_0$  and satisfy

$$|g(x) - g_{x_0}^{(\beta)}(x)| \leq L \|x - x_0\|_2^\beta, \quad \forall x \in \mathcal{B}_\infty(x_0, r),$$

for some  $r > 0$ . The set  $\Sigma(\beta, L, x_0)$  is called  $(\beta, L, x_0)$ -locally Hölder class of functions.

We now define the class of densities that are considered in this paper.

**Definition 2.2** Fix  $\beta > 0, L > 0, \lambda > 0$  and  $\gamma \geq 0$ . Let  $\mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)$  denote the class of all probability densities  $p$  on  $\mathcal{X}$  such that

- (i)  $\exists \eta > 0$  such that  $p \in \Sigma(\beta, L, x_0)$  for all  $x_0 \in \mathcal{D}(\eta) = p^{-1}([\lambda - \eta, \lambda + \eta])$ , apart from a set of null measure  $Q$ .
- (ii)  $\exists \beta' > 0$  such that  $p \in \Sigma(\beta', L, x_0)$ , for all  $x_0 \notin \mathcal{D}(\eta)$ , apart from a set of null measure  $Q$ .
- (iii)  $p$  has  $\gamma$ -exponent at level  $\lambda$  with respect to  $Q$ .
- (iv)  $p$  is uniformly bounded by a constant  $L^*$ .

The class  $\mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)$  is the class of uniformly bounded (condition (iv)) densities that have  $\gamma$ -exponent at level  $\lambda$  with respect to  $Q$  (condition (iii)) and that are smooth in the neighborhood of the level under consideration (condition (i)). Remark that the parameters  $\beta'$  in condition (ii) and  $L^*$  in condition (iv) do not appear in the notation of the class. Indeed  $\beta' > 0$  can be arbitrary close to 0 and this will not affect the rates of convergence. Actually, the role of condition (ii) is to ensure that any density from the class can be consistently estimated at any point with an arbitrary slow polynomial rate. In the same manner, the constant  $L^*$  does not appear in the rates of convergence and only affects the constants.

To estimate a density from this class we can use a *kernel density estimator* defined by:

$$\hat{p}_n(x) = \hat{p}_{n,h}(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right), \quad (2.2)$$

where  $h > 0$  is the bandwidth parameter and  $K : \mathcal{X} \rightarrow \mathbb{R}$  is a kernel. In the sequel, a specific family of kernels is considered.

**Definition 2.3** Let  $K$  be a real-valued function on  $\mathbb{R}^d$ , with support  $[-1, 1]^d$ . Fix  $\beta > 0$ , and let  $\lfloor \beta \rfloor$  denote the maximal integer that is strictly less than  $\beta$ . The function  $K(\cdot)$  is said to be a  $\beta$ -valid kernel if it satisfies  $\int K = 1$ ,  $\int |K|^p < \infty$  for any  $p \geq 1$ ,  $\int \|t\|_2^\beta |K(t)| dt < \infty$ , and, in case  $\lfloor \beta \rfloor \geq 1$ , it satisfies  $\int t^s K(t) dt = 0$  for any  $s = (s_1, \dots, s_d) \in \mathbb{N}^d$  such that  $1 \leq s_1 + \dots + s_d \leq \lfloor \beta \rfloor$ .

**Example 2.1** Let  $\beta > 0$ . For any  $\beta$ -valid kernel  $K$  defined on  $\mathbb{R}^d$ , consider the following product kernel

$$\tilde{K}(x) = K(x_1)K(x_2) \dots K(x_d) \mathbb{1}_{x \in [-1, 1]^d},$$

for any  $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ . Then it can be easily shown that  $\tilde{K}$  is a  $\beta$ -valid kernel on  $\mathbb{R}^d$ . Now, for any  $\beta > 0$ , an example of a 1-dimensional  $\beta$ -valid kernel is given in (Tsybakov, 2004a, section 1.2.2), the construction of which is based on Legendre polynomials. This eventually proves the existence of a multivariate  $\beta$ -valid kernel, for any given  $\beta > 0$ .

The following proposition holds.

**Proposition 2.2** Fix  $\beta > 0$ . If  $K$  is a  $\beta$ -valid kernel, then  $K$  is also a  $\beta'$ -valid kernel for any  $0 < \beta' \leq \beta$ .

PROOF. Fix  $\beta$  and  $\beta'$  such that  $0 < \beta' \leq \beta$ . Remark that  $\lfloor \beta' \rfloor \leq \lfloor \beta \rfloor$ . For any  $\beta$ -valid kernel  $K$ , we have  $\int t^s K(t) dt = 0$  for any  $s = (s_1, \dots, s_d)$  such that  $1 \leq s_1 + \dots + s_d \leq \lfloor \beta' \rfloor$ . It remains to check that

$$\int_{\mathbb{R}^d} \|t\|_2^{\beta'} |K(t)| dt < \infty. \quad (2.3)$$

Consider the decomposition

$$\begin{aligned} \int_{\mathbb{R}^d} \|t\|_2^{\beta'} |K(t)| dt &= \int_{\|t\|_2 \leq 1} \|t\|_2^{\beta'} |K(t)| dt + \int_{\|t\|_2 \geq 1} \|t\|_2^{\beta'} |K(t)| dt \\ &\leq \int_{\mathbb{R}^d} |K(t)| dt + \int_{\|t\|_2 \geq 1} \|t\|_2^\beta |K(t)| dt. \end{aligned}$$

To prove (2.3), remark that since  $K$  is a  $\beta$ -valid kernel, we have  $\int_{\mathbb{R}^d} |K(t)| dt < \infty$  and

$$\int_{\|t\|_2 \geq 1} \|t\|_2^\beta |K(t)| dt \leq \int_{\mathbb{R}^d} \|t\|_2^\beta |K(t)| dt < \infty.$$

■

Intuitively, parameters  $\gamma$  and  $\beta$  are conflicting. Indeed, the parameter  $\beta$  ensures that the density  $p$  has a relatively small slope around level  $\lambda$  and the parameter  $\gamma$  requires  $p$  to have a slope that is not too small around level  $\lambda$ . The following proposition gives an explicit constraint on the possible parameters  $\gamma$  and  $\beta$ .

**Proposition 2.3** *When  $Q$  is the Lebesgue measure  $\text{Leb}_d$ , if  $\gamma(1 \wedge \beta) > d$ , there is no density  $p \in \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)$  such that  $\lambda$  is in the interior of  $p(\mathcal{X})$ .*

PROOF. Let  $p$  be a density in  $\mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)$  with  $\lambda$  in the interior of  $p(\mathcal{X})$ . There exists  $x_0$  such that  $p(x_0) = \lambda$  and for any  $x$  in a neighborhood of  $x_0$  we can decompose

$$|p(x) - \lambda| \leq |p(x) - p_{x_0}^{(\beta)}(x)| + |p_{x_0}^{(\beta)}(x) - \lambda|.$$

Since  $p$  is  $(\beta, L, x_0)$ -locally Hölder the first term can be bounded from above by  $L\|x - x_0\|_2^\beta$ . Now, if  $\beta \leq 1$ , the second term is null. If  $\beta > 1$ , this term is a polynomial of degree  $\lfloor \beta \rfloor \geq 1$  with no constant term. Hence

$$|p_{x_0}^{(\beta)}(x) - \lambda| = |p_{x_0}^{(\beta)}(x) - p(x_0)| \leq c_2 \max_{1 \leq j \leq d} |x^{(j)} - x_0^{(j)}| \leq c_2 \|x - x_0\|_2.$$

Since  $\beta > 1$  and  $\|x - x_0\|_2$  is bounded by a constant,  $\|x - x_0\|_2^\beta \leq c_3 \|x - x_0\|_2$ . Thus, for any  $\beta > 0$ , if  $p$  has  $\gamma$ -exponent at level  $\lambda$  with respect to  $Q$ ,

$$c\varepsilon^\gamma \geq Q(x : |p(x) - \lambda| \leq \varepsilon) \geq Q(x : c_4 \|x - x_0\|_2^{\beta \wedge 1} \leq \varepsilon) \geq c_5 \varepsilon^{d/(\beta \wedge 1)}.$$

■

### 3 Fast rates for penalized plug-in rules

The first theorem states that rates of convergence for penalized plug-in rules can be obtained using exponential inequalities for the corresponding non-parametric density estimator  $\hat{p}_n$ . For any measurable function  $f$  on  $\mathcal{X}$  and any set  $A \subset f(\mathcal{X})$ , we write for simplicity  $\{x \in \mathcal{X} : f(x) \in A\} = \{f \in A\}$ .

**Theorem 3.1** Fix  $\lambda > 0$  and  $\Delta > 0$ . Let  $\hat{p}_n$  be an estimator of the density  $p$  such that  $Q(\hat{p}_n \geq \lambda) \leq C$ , almost surely for some positive constant  $C$  and let  $\mathcal{P}$  be class of densities on  $\mathcal{X}$ . Assume that there exists positive constants  $\eta, c_6, c_7, c_8, c_9, c_\delta, c'_\delta, a$  and  $b$ , such that

- for  $Q$ -almost all  $x \in \mathcal{D}(\eta) = p^{-1}([\lambda - \eta, \lambda + \eta])$  and for any  $\delta$  such that  $c_\delta n^{-a/2} < \delta < \Delta$ , we have

$$\sup_{p \in \mathcal{P}} \mathbb{P} (|\hat{p}_n(x) - p(x)| \geq \delta) \leq c_6 e^{-c_7 n^a \delta^2}, \quad n \geq 1. \quad (3.1)$$

- and for  $Q$ -almost all  $x \in \mathcal{X} \setminus \mathcal{D}(\eta)$ , for any  $\delta$  such that  $c'_\delta n^{-b/2} \leq \delta \leq \Delta$ , we have

$$\sup_{p \in \mathcal{P}} \mathbb{P} (|\hat{p}_n(x) - p(x)| \geq \delta) \leq c_8 e^{-c_9 n^a \delta^2}, \quad n \geq 1. \quad (3.2)$$

Then if  $p$  has  $\gamma$ -exponent at level  $\lambda$  for any  $p \in \mathcal{P}$  and if  $\ell_n = O(n^{-a/2})$ , the following upper bound holds,

$$\sup_{p \in \mathcal{P}} \mathbb{E} \left[ d_H(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] \leq c_{10} n^{-\frac{(1+\gamma)a}{2}}, \quad (3.3)$$

$$\sup_{p \in \mathcal{P}} \mathbb{E} \left[ d_\Delta(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] \leq c_{11} n^{-\frac{\gamma a}{2}}, \quad (3.4)$$

for  $n \geq n_0 = n_0(\lambda, \eta, a, b, \varepsilon_0, c_\delta, c'_\delta)$  and where  $c_{10} > 0$  and  $c_{11} > 0$  depend only on  $c_6, c_7, c_8, c_9, C, a, b, \gamma$  and  $\lambda$ .

PROOF. Note first that the conditions of Proposition 2.1 are satisfied. Indeed,  $Q(\hat{p}_n \geq \lambda) + Q(p \geq \lambda) \leq C + \lambda^{-1}$  and we choose  $L_Q = C + \lambda^{-1}$ . Therefore, (3.4) is a direct consequence of (3.3) and we prove the latter using the same scheme as in the proof of Audibert and Tsybakov (2005, Theorem 3.1).

Recall that  $\tilde{\Gamma}_{\ell_n} \triangleq \Gamma = (\tilde{\Gamma}_{\ell_n} \cap \Gamma^c) \cup (\tilde{\Gamma}_{\ell_n}^c \cap \Gamma)$ . It yields

$$\mathbb{E} \left[ d_H(\Gamma, \tilde{\Gamma}_{\ell_n}) \right] = \mathbb{E} \int_{\tilde{\Gamma}_{\ell_n} \cap \Gamma^c} |p(x) - \lambda| dQ(x) + \mathbb{E} \int_{\tilde{\Gamma}_{\ell_n}^c \cap \Gamma} |p(x) - \lambda| dQ(x).$$

Define two sequences

$$\ell_n^a = n^{-a/2} \quad \text{and} \quad \ell_n^b = \left( \frac{2c_9 n^{a \wedge b}}{(1+\gamma)a \log n} \right)^{-1/2}.$$

Let  $n_0$  be a positive integer such that  $\ell_n^a < \ell_n^b < \min(\eta, \varepsilon_0) = r$  and  $\ell_n^b > c'_\delta n^{-b/2}$  for all  $n \geq n_0$ . Recall that  $\mathcal{D}(r) = p^{-1}([\lambda - r, \lambda + r])$ . Consider the following decomposition:

$$\tilde{\Gamma}_{\ell_n} \cap \Gamma^c = \{\hat{p}_n \geq \lambda + \ell_n, p < \lambda\} = A_1 \cup A_2 \cup A_3, \quad (3.5)$$

where,

$$\begin{aligned} A_1 &= \{\hat{p}_n \geq \lambda + \ell_n, \lambda - \ell_n^a \leq p < \lambda\}, \\ A_2 &= \{\hat{p}_n \geq \lambda + \ell_n, \lambda - \ell_n^b \leq p < \lambda - \ell_n^a\}, \\ A_3 &= \{\hat{p}_n \geq \lambda + \ell_n, p < \lambda - \ell_n^b\}. \end{aligned}$$

Remark that  $A_1 \subseteq \{|p - \lambda| \leq \ell_n^a\}$ . It yields for  $n \geq n_0$ ,

$$\mathbb{E} \int_{A_1} |p(x) - \lambda| dQ(x) \leq \ell_n^a Q(A_1) \leq c_0 (\ell_n^a)^{1+\gamma} = c_0 n^{-\frac{(1+\gamma)a}{2}}, \quad (3.6)$$

where in the last inequality we used the  $\gamma$ -exponent of  $p$ . Then when  $n \geq n_0$ , we can decompose  $A_2$  into the disjoint union:

$$A_2 = \bigcup_{j=1}^{\infty} \mathcal{X}_j, \quad \mathcal{X}_j = \{\hat{p}_n \geq \lambda + \ell_n, \lambda - 2^j \ell_n^a \leq p < \lambda - 2^{j-1} \ell_n^a\} \cap \mathcal{D}(r).$$

Hence,

$$\mathbb{E} \int_{A_2} |p(x) - \lambda| dQ(x) = \sum_{j=1}^{\infty} \mathbb{E} \int_{\mathcal{X}_j} |p(x) - \lambda| dQ(x). \quad (3.7)$$

Using the Fubini Theorem, the general term of the sum in the right-hand side of (3.7) can be bounded from above by

$$2^j \ell_n^a \int_{\mathcal{D}(r)} \mathbb{P} [|\hat{p}_n(x) - p(x)| > 2^{j-1} \ell_n^a] \mathbb{1}_{\{|p(x) - \lambda| < 2^j \ell_n^a\}} dQ(x).$$

Using now (3.1) and the fact that  $p$  has  $\gamma$ -exponent at level  $\lambda$ , we get

$$\begin{aligned} \mathbb{E} \int_{A_2} |p(x) - \lambda| dQ(x) &\leq c_0 c_6 \sum_{j \geq 1} \exp(-c_7 n^a (2^{j-1} \ell_n^a)^2) (2^j \ell_n^a)^{1+\gamma} \\ &\leq c_{12} (\ell_n^a)^{1+\gamma} = c_{12} n^{-\frac{(1+\gamma)a}{2}}. \end{aligned} \quad (3.8)$$

We now treat the integral over  $A_3$  using the Fubini theorem and the assumption  $Q(\hat{p}_n \geq \lambda) \leq C$ , a.s.

$$\begin{aligned} \mathbb{E} \int_{A_3} |p(x) - \lambda| dQ(x) &\leq \sup_{\substack{G \subseteq \mathcal{X} \\ Q(G) \leq C}} \int_G |p(x) - \lambda| \mathbb{P} \left[ |\hat{p}_n(x) - p(x)| > \ell_n^b \right] dQ(x) \\ &\leq (1 + \lambda C) c_8 \exp \left( -c_9 n^a (\ell_n^b)^2 \right) \leq c_{13} n^{-\frac{(1+\gamma)a}{2}}, \end{aligned} \quad (3.9)$$

where in the last inequality, we used the fact that

$$\ell_n^b \geq \left( \frac{2c_4 n^a}{(1 + \gamma)a \log n} \right)^{-1/2}.$$

In view of (3.5), if we combine (3.6), (3.8) and (3.9), we obtain

$$\mathbb{E} \int_{\tilde{\Gamma}_{\ell_n} \cap \Gamma^c} |p(x) - \lambda| dQ(x) \leq c_{14} n^{-\frac{(1+\gamma)a}{2}},$$

where  $c_{14}$  depends on  $c_6, c_7, c_8, c_9, C, a, b, \gamma$  and  $\lambda$ . In the same manner, using the fact that  $\ell_n \leq c_{15} \ell_n^a$ , it can be shown that for  $n \geq n_0$ ,

$$\mathbb{E} \int_{\tilde{\Gamma}_{\ell_n}^c \cap \Gamma} |p(x) - \lambda| dQ(x) \leq c_{16} n^{-\frac{(1+\gamma)a}{2}}.$$

where  $c_{16}$  depends on  $c_6, c_7, c_8, c_9, a, b, \gamma, \lambda$  but not on  $C$ . ■

**Remark 3.1** *If  $\ell_n > 0$ , i.e., we use penalized plug-in rules, we get*

$$\begin{aligned} \mathbb{E} Q(\tilde{\Gamma}_{\ell_n} \cap \Gamma^c) &= \mathbb{E} \int_{\tilde{\Gamma}_{\ell_n} \cap \Gamma^c} dQ(x) \\ &\leq \sup_{\substack{G \subseteq \mathcal{X} \\ Q(G) \leq C}} \int_G \mathbb{P} [|\hat{p}_n(x) - p(x)| > \ell_n] dQ(x) \\ &\leq c_{6,8} C \exp \left( -c_{7,9} n^a \ell_n^2 \right), \end{aligned}$$

where  $c_{6,8} \in \{c_6, c_8\}$  and  $c_{7,9} \in \{c_7, c_9\}$ . Thus the choice

$$\ell_n = \left( \frac{c_{7,9} n^a}{\alpha \log n} \right)^{-1/2}, \quad \alpha > 0,$$

yields

$$\mathbb{E}Q(\tilde{\Gamma}_{\ell_n} \cap \Gamma^c) = O(n^{-\alpha}),$$

whatever is  $\gamma \geq 0$ . This is of particular interest if  $\gamma$  is very small. Indeed, even in such cases we might be interested in the situation where the density level set estimator is included in the density level set to be estimated with high probability. Note that for such a choice of  $\ell_n$ , the resulting performance of the density level set estimator is only altered by a logarithmic factor. Indeed we have

$$\begin{aligned} \sup_{p \in \mathcal{P}} \mathbb{E} \left[ d_H(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] &\leq c_{17} \left( \frac{n^a}{\log n} \right)^{-(1+\gamma)/2}, \\ \sup_{p \in \mathcal{P}} \mathbb{E} \left[ d_{\Delta}(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] &\leq c_{18} \left( \frac{n^a}{\log n} \right)^{-\gamma/2}. \end{aligned}$$

When the density  $p$  belongs to the class  $\mathcal{P}_{\Sigma}(\beta, L, \lambda, \gamma)$ , a kernel density estimator defined in (2.2) can be used to obtain exponential inequalities as in (3.1) and (3.2). This choice is not the only possible one.

**Lemma 3.1** *Let  $P$  be a distribution on  $\mathbb{R}^d$  having a density  $p$  w.r.t. the measure  $Q$  such that  $\|p\|_{\infty} \leq L^*$  for some constant  $L^* > 0$ . Fix  $\beta > 0$ ,  $\beta^* \geq \beta$ ,  $L > 0$  and assume that  $p \in \Sigma(\beta, L, x_0)$  ( $\beta, L, x_0$ )-locally Hölder class of functions where the neighborhood around  $x_0$  is a ball of radius  $r > 0$ . Let  $\hat{p}_n$  be a kernel density estimator with bandwidth  $h > 0$  and  $\beta^*$ -valid kernel  $K$ , given an i.i.d. sample  $X_1, \dots, X_n$  from  $P$ :*

$$\hat{p}_n(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right).$$

Set

$$\Delta = \frac{6L^*\|K\|^2}{\|K\|_{\infty} + L^* + L \int \|t\|_2^{\beta} K(t) dt}.$$

Then, for all  $\delta, h \leq r$  such that  $\Delta > \delta > 2Lc_{19}h^{\beta} > 0$ , we have,

$$\mathbb{P}\{|\hat{p}_n(x_0) - p(x_0)| \geq \delta\} \leq 2 \exp\left(-c_{20}nh^d\delta^2\right),$$

where  $c_{19} = \int \|t\|_2^{\beta} K(t) dt$  and  $c_{20} = 1/(16L^*\|K\|^2)$ .

PROOF. For any  $x_0 \in \mathbb{R}^d$ ,

$$|\hat{p}_n(x_0) - p(x_0)| \leq \frac{1}{n} \left| \sum_{i=1}^n Z_i(x_0) \right|,$$



with

$$Z_i(x) = \frac{1}{h^d} K\left(\frac{X_i - x}{h}\right) - p(x).$$

The expectation of  $Z_i(x_0)$  is the pointwise bias of a kernel density estimator with bandwidth  $h$ . Under the assumptions of the theorem, it is controlled in the following way

$$|\mathbb{E}Z_i(x_0)| \leq Lc_{19}h^\beta.$$

Indeed,

$$\begin{aligned} |\mathbb{E}Z_i(x_0)| &= \\ &= \left| \int \frac{1}{h^d} K\left(\frac{t}{h}\right) [p(x_0 + t) - p(x_0)] dt \right| \\ &= \left| \int K(t) [p(x_0 + ht) - p(x_0)] dt \right| \\ &= \left| \int K(t) [p(x_0 + ht) - p_{x_0}^{(\beta)}(x_0 + ht)] dt + \int K(t) [p_{x_0}^{(\beta)}(x_0 + ht) - p(x_0)] dt \right| \end{aligned} \tag{3.10}$$

To control the first term in the RHS of (3.10), remark that since  $K$  has support  $[-1, 1]^d$ , for any  $h < r$ , we have  $x_0 + ht \in \mathcal{B}_\infty(x_0, r)$  for any  $t \in [-1, 1]^d$ . Thus, using the fact that  $p$  is in  $\Sigma(\beta, L, x_0)$  we have

$$\left| \int K(t) [p(x_0 + ht) - p_{x_0}^{(\beta)}(x_0 + ht)] dt \right| \leq L \int |K(t)| \|ht\|_2^\beta dt.$$

Now, since  $K$  is a kernel of order  $[\beta]$  (cf. Proposition 2.2) and  $p_{x_0}^{(\beta)} - p(x_0)$  is a polynomial of degree at most  $[\beta]$  with no constant term, the second term in the RHS of (3.10) is zero. Therefore, it holds

$$|\mathbb{E}Z_i(x_0)| \leq Lh^\beta \int |K(t)| \|t\|_2^\beta dt, \quad \text{for any } h \leq r$$

Now denote for simplicity  $Z_i = Z_i(x_0)$  and let  $\overline{Z}_i$  be the centered version of  $Z_i$ . Then, when  $Lc_{19}h^\beta \leq \delta/2$ ,

$$\begin{aligned} \mathbb{P}\{|\hat{p}_n(x_0) - p(x_0)| \geq \delta\} &\leq \mathbb{P}\left\{\frac{1}{n} \left| \sum_{i=1}^n \overline{Z}_i \right| \geq \delta - Lc_{19}h^\beta\right\} \\ &\leq \mathbb{P}\left\{\frac{1}{n} \left| \sum_{i=1}^n \overline{Z}_i \right| \geq \frac{\delta}{2}\right\}. \end{aligned}$$

The right-hand side of the last inequality can be bounded applying Bernstein's inequality to  $\overline{Z}_i$  and  $-\overline{Z}_i$  successively. For  $h \geq 1$ , one has

$$|\overline{Z}_i| \leq \|K\|_\infty h^{-d} + L^* + Lc_{19}h^\beta \leq c_{21}h^{-d},$$

where  $c_{21} = \|K\|_\infty + L^* + Lc_{19}$  and

$$\text{Var}\{Z_i\} \leq h^{-d} \int K(u)^2 p(hu) du \leq c_{22}h^{-d},$$

where  $c_{22} = L^*\|K\|^2$ . Applying now Bernstein's inequality yields

$$\begin{aligned} \mathbb{P}\{|\hat{p}_n(x_0) - p(x_0)| \geq \delta\} &\leq 2 \exp\left(-\frac{n(\delta/2)^2}{2(c_{22}h^{-d} + c_{21}h^{-d}\delta/6)}\right) \\ &\leq 2 \exp\left(-c_{20}nh^d\delta^2\right), \end{aligned}$$

for any  $\delta \leq \Delta$  and where  $\Delta = 6c_{22}/c_{21}$  and  $c_{20} = 1/(16c_{22})$ .  $\blacksquare$

We can therefore apply Theorem 3.1. When the choice of  $h$  is optimal, i.e.,  $h = n^{-1/(2\beta+d)}$ , it yields the following corollary.

**Corollary 3.1** *Fix  $\beta > 0$ ,  $L > 0$ ,  $\lambda > 0$ ,  $\gamma > 0$  and consider the penalized plug-in estimator  $\tilde{\Gamma}_{\ell_n}$ , where  $0 \leq \ell_n \leq c_{15}n^{-\beta/(2\beta+d)}$ ,  $c_{15} > 0$ . The nonparametric estimator  $\hat{p}_n$  is the kernel density estimator defined in (2.2) with bandwidth parameter  $h = n^{-1/(2\beta+d)}$  and  $\beta^*$ -valid kernel  $K$ , where  $\beta^* = \max(\beta, \beta')$  and  $\beta'$  is the parameter from Definition 2.2. Then,*

$$\begin{aligned} \sup_{p \in \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)} \mathbb{E} \left[ d_H(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] &\leq c_{23}n^{-\frac{(1+\gamma)\beta}{2\beta+d}}, \\ \sup_{p \in \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)} \mathbb{E} \left[ d_\Delta(\Gamma_p(\lambda), \tilde{\Gamma}_{\ell_n}) \right] &\leq c_{24}n^{-\frac{\gamma\beta}{2\beta+d}}, \end{aligned}$$

where  $c_{23} > 0$  and  $c_{24} > 0$  depend on the constants  $c_{19}$  and  $c_{20}$  that appear in Lemma 3.1, on  $c_0, \beta, \beta', \gamma, d$  and on  $\lambda$ .

PROOF. The results are direct consequences of Theorem 3.1 when  $\hat{p}_n$  is chosen as in (2.2). We need to check that for such an estimator we have  $Q(\hat{p}_n \geq \lambda) \leq C$ , almost surely for some  $C > 0$ . Note that since  $K \in L_1(\mathbb{R}^d)$ , we have

$$\infty > \int_{\mathbb{R}^d} |K(x)| dQ(x) \geq \int_{\{\hat{p}_n \geq \lambda\}} |\hat{p}_n(x)| dQ(x) \geq \lambda Q\{\hat{p}_n \geq \lambda\}.$$

Hence, the condition is satisfied with  $C = \lambda^{-1} \int |K|$ . All the other conditions of Theorem 3.1 are satisfied and we can apply it with  $a = 2\beta/(2\beta + d)$  and  $b = 2\beta'/(2\beta + d)$ .  $\blacksquare$

## 4 Minimax lower bounds

The following theorem shows that the rate obtained in Corollary 3.1 is optimal in a minimax sense.

**Theorem 4.1** *Assume that  $Q$  is the Lebesgue measure on  $\mathcal{X}$ . Fix  $\lambda > 0$  and let  $L, \beta, \gamma$  be positive constants such that  $\gamma\beta \leq d$ . Then, there exists constants  $c_{25} > 0$  and  $c_{26} > 0$  such that for any  $n \geq 1$  and any estimator  $\hat{G}_n$  of  $\Gamma_p(\lambda)$  constructed from the sample  $X_1, \dots, X_n$ , we have*

$$\begin{aligned} \sup_{p \in \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)} \mathbb{E} \left[ d_H(\Gamma_p(\lambda), \hat{G}_n) \right] &\geq c_{25} n^{-\frac{(1+\gamma)\beta}{2\beta+d}}, \\ \sup_{p \in \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)} \mathbb{E} \left[ d_\Delta(\Gamma_p(\lambda), \hat{G}_n) \right] &\geq c_{26} n^{-\frac{\gamma\beta}{2\beta+d}}. \end{aligned} \quad (4.1)$$

PROOF. In view of Proposition 2.1, we only have to prove (4.1). To that end, we will use Lemma 5.2 with  $d = d_\Delta$ ,  $\varepsilon = \varepsilon_n \sim n^{-\frac{\gamma\beta}{2\beta+d}}$  and  $\mathcal{P} = \mathcal{P}_\Sigma(\beta, L, \lambda, \gamma)$ . Assume without loss of generality that  $\lambda = 1$ .

We now describe the construction of the family  $\mathcal{N}$ . Define the support density by

$$p_0(x) = \begin{cases} 1 & \text{if } 0 \leq x^{(j)} \leq 1, \text{ for any } j = 1, \dots, d, \\ 0 & \text{else.} \end{cases}$$

We now define perturbations of the support density. Consider the integer  $q = \lfloor c_{27} n^{\frac{1}{2\beta+d}} \rfloor$  where  $c_{27}$  is a positive constant chosen large enough to ensure that  $q \geq 1$ , and the regular grid  $\mathcal{G}$  on  $[0, 1]^d$  defined as

$$\mathcal{G} = \left\{ \left( \frac{2k_1 + 1}{2q}, \dots, \frac{2k_d + 1}{2q} \right), k_i \in \{0, \dots, q-1\}, i = 1, \dots, d \right\}.$$

Re-index the grid by  $\mathcal{G} = \{g_j\}_{1 \leq j \leq q^d}$  and define the integer  $m = \lfloor c_{28} q^{d-\gamma\beta} \rfloor$  for some positive constant  $c_{28}$ . The condition  $\gamma\beta \leq d$  ensures that  $m \geq 2$  if  $c_{28}$  is chosen large enough. Let  $\mathcal{J} = \{1, 3, \dots, 2m-1\}$  be the set of odd integers between 1 and  $2m-1$  and for any  $j = 1, \dots, 2m$ , define the disjoint balls  $B_j = \mathcal{B}_{\tilde{\beta}}(g_j, (4q)^{-1})$ , where  $\tilde{\beta} = \beta$  if  $\beta > 1$  and  $\tilde{\beta} = 2$  if  $\beta < 1$ . Set  $B_0 = [0, 1]^d \setminus \bigcup_{j=1}^{2m} B_j$  and consider a partition of  $B_0$  into two measurable sets  $B_0 = C_1 \cup C_2$  such that  $Q(C_1) = Q(C_2) = Q(B_0)/2$ . For any  $j \in \mathcal{J}$ , define the function  $\varphi_j$  on  $[0, 1]^d$  by

$$\varphi_j(x) = \tilde{L} \|x - g_j\|_{\tilde{\beta}}^\beta \mathbb{1}_{\{x \in B_j\}} - \tilde{L} \|x - g_{j+1}\|_{\tilde{\beta}}^\beta \mathbb{1}_{\{x \in B_{j+1}\}}, \quad 0 < \tilde{L} < 1.$$

For any  $\omega = (\omega_1, \dots, \omega_m) \in \{-1, 1\}^m$ , define the density

$$p_\omega(x) = 1 + \sum_{j \in \mathcal{J}} \omega_j \varphi_j(x) + \kappa (\mathbb{I}_{\{x \in C_1\}} - \mathbb{I}_{\{x \in C_2\}}) ,$$

where  $\kappa < 1$  is a tuning parameter. Consider a set  $\Omega \subset \{-1, 1\}^m$  of cardinality  $s$  and define the family  $\mathcal{N}$  as

$$\mathcal{N} = \{p_\omega, \omega \in \Omega\} .$$

The tuning parameters,  $\tilde{L}$ ,  $\kappa$  and  $\Omega$ , will be chosen in order to fulfill the conditions of Lemma 5.2.

FIRST CONDITION:  $\mathcal{N} \subset \mathcal{P}_\Sigma(\beta, L, 1, \gamma)$ .

Remark first that for any  $\omega \in \Omega$ ,  $p_\omega$  is a density that satisfies  $\|p_\omega\|_\infty \leq 2$ . Next, fix  $\eta > 0$  and  $x_0 \in \mathcal{D}(\eta) = p_\omega^{-1}\{[1 - \eta, 1 + \eta]\}$  outside of the set of null Lebesgue measure where  $p_\omega$  is not differentiable. If  $x_0$  is in the interior of  $B_0$  then  $p$  is constant in a neighborhood of  $x_0$  and obviously belongs to  $\Sigma(\beta, L, x_0)$ . Fix  $j \in \{1, \dots, 2m\}$  and assume that  $x_0 \in B_j, x_0 \neq g_j$ , for some  $j = 1, \dots, 2m$ .

We begin by treating the case  $\beta > 1$ . For any  $x \in B_j$ , we have

$$p_\omega(x) = 1 + \sigma_j \tilde{L} \sum_{l=1}^d |x^{(l)} - g_j^{(l)}|^\beta ,$$

where  $\sigma_j \in \{-1, 1\}$ . Fix  $l \in \{1, 2, \dots, d\}$ , and assume without loss of generality that  $x_0^{(l)} > g_j^{(l)}$ . Consider now a real number  $x^{(l)}$  such that  $|x^{(l)} - x_0^{(l)}| \leq (x_0^{(l)} - g_j^{(l)})/2$ . A Laplace-Taylor expansion at point  $x_0^{(l)}$  gives

$$|x^{(l)} - g_j^{(l)}|^\beta = \sum_{k=0}^{\lfloor \beta \rfloor} C(k, \beta) (x^{(l)} - x_0^{(l)})^k (x_0^{(l)} - g_j^{(l)})^{\beta-k} + R^{(l)} ,$$

where  $C(k, \beta) \neq 0$  depends only on  $\beta, k$  and the sign of  $x^{(l)} - g_j^{(l)}$ . The residual term is given by

$$R^{(l)} = C'(\beta) \int_{x_0^{(l)}}^{x^{(l)}} (x^{(l)} - t)^{\lfloor \beta \rfloor} (t - g_j^{(l)})^{\beta - \lfloor \beta \rfloor - 1} dt ,$$

where  $C'(\beta)$  depends only on  $\beta$  and the sign of  $x^{(l)} - g_j^{(l)}$ . Note now that since  $\beta - \lfloor \beta \rfloor - 1 \leq 0$ , we have

$$|R^{(l)}| \leq |C'(\beta)| |x^{(l)} - x_0^{(l)}|^\beta .$$

Summing up over  $l$  allows us to bound from above the difference between  $p_\omega$  and its Taylor polynomial of degree  $\lfloor \beta \rfloor$  at point  $x_0$  by the quantity

$$c_{29}\tilde{L}\|x - x_0\|_\beta^\beta \leq c_{30}\tilde{L}\|x - x_0\|_2^\beta,$$

where  $c_{29}$  and  $c_{30}$  are positive constants that depend only on  $\beta$  and  $d$ .

When  $\beta \leq 1$ ,  $\tilde{\beta} = 2$  and the Taylor polynomial of  $p_\omega$  at point  $x_0$  has degree  $\lfloor \beta \rfloor = 0$ . Therefore, it is constant and equals  $p_\omega(x_0)$ . It yields

$$\begin{aligned} |p_\omega(x) - p_\omega(x_0)| &= \tilde{L} \left| \|x - g_j\|_2^\beta - \|x_0 - g_j\|_2^\beta \right| \\ &\leq \tilde{L} \left| \|x - g_j\|_2 - \|x_0 - g_j\|_2 \right|^\beta \\ &\leq \tilde{L} \|x - x_0\|_2^\beta. \end{aligned}$$

For any  $\beta > 0$ , taking  $\tilde{L}$  such that  $c_{30}\tilde{L} \leq L \wedge 1/2$ , yields that  $\mathcal{N} \subset \Sigma(\beta, L, x_0)$ .

For large enough  $\eta$ ,  $\mathcal{D}(\eta) = [0, 1]^d$  and we can take  $\beta' = \beta$  in condition (ii). Therefore we only have to check that  $p_\omega$  has  $\gamma$ -exponent at level 1 with respect to the Lebesgue measure. The following decomposition holds:

$$\begin{aligned} Q(x : |p - 1| \leq \varepsilon) &= 2 \sum_{j \in \mathcal{J}} Q(x : |p(x) - 1| \leq \varepsilon, x \in B_j) \\ &\quad + Q(x : |p(x) - 1| \leq \varepsilon, x \in B_0) \\ &= 2mQ(x : |p(x) - 1| \leq \varepsilon, x \in B_1) + Q(B_0)\mathbb{I}_{\{\varepsilon \geq \kappa\}}. \end{aligned} \tag{4.2}$$

We have on the one hand,

$$mQ(x : |p(x) - 1| \leq \varepsilon, x \in B_1) \leq c_{31}mq^{-d}\mathbb{I}_{\{\varepsilon \geq \tilde{L}q^{-\beta}\}} + c_{32}m\varepsilon^{d/\beta}\mathbb{I}_{\{\varepsilon < \tilde{L}q^{-\beta}\}}.$$

Since  $m \leq c_{28}q^{d-\gamma\beta}$  we have  $mq^{-d} \leq c_{28}q^{-\gamma\beta}$ . It yields

$$mq^{-d}\mathbb{I}_{\{\varepsilon \geq \tilde{L}q^{-\beta}\}} \leq c_{28}q^{-\gamma\beta}\mathbb{I}_{\{\varepsilon^\gamma \geq \tilde{L}q^{-\gamma\beta}\}} \leq c_{33}\varepsilon^\gamma,$$

and

$$m\varepsilon^{d/\beta}\mathbb{I}_{\{\varepsilon < \tilde{L}q^{-\beta}\}} \leq c_{28}q^{d-\gamma\beta}\varepsilon^{d/\beta}\mathbb{I}_{\{q^{d-\gamma\beta} < (\varepsilon/\tilde{L})^{\gamma-d/\beta}\}} \leq c_{34}\varepsilon^\gamma.$$

Therefore

$$mQ(x : |p(x) - 1| \leq \varepsilon, x \in B_1) \leq c_{35}\varepsilon^\gamma. \tag{4.3}$$

On the other hand,

$$Q(B_0)\mathbb{I}_{\{\varepsilon \geq \kappa\}} = (1 - c_{36}mq^{-d})\mathbb{I}_{\{\varepsilon \geq \kappa\}} \leq c_{37}\varepsilon^\gamma, \tag{4.4}$$

when  $\kappa = c_{38}(1 - c_{36}mq^{-d})^{1/\gamma} < 1$ . Equation (4.2) together with (4.3) and (4.4) yield

$$Q(x : |p - 1| \leq \varepsilon) \leq c_{39}\varepsilon^\gamma.$$

for  $\kappa = c_{38}(1 - c_{36}mq^{-d})^{1/\gamma}$ .

SECOND CONDITION (5.1):  $d_\Delta(\Gamma_p, \Gamma_q) \geq \varepsilon_n, \forall p, q \in \mathcal{N}, p \neq q$ .

By construction, for any  $\omega, \omega' \in \{-1, 1\}^m$ ,

$$d_\Delta(\Gamma_{p_\omega}, \Gamma_{p_{\omega'}}) = 2 \sum_{j=1}^m \mathbb{I}_{\{\omega_j \neq \omega'_j\}} q^{-d}.$$

We need to bound from below the Hamming distance between  $\omega$  and  $\omega'$ , defined for any  $\omega, \omega' \in \Omega$  by

$$\rho(\omega, \omega') = \sum_{j=1}^m \mathbb{I}_{\{\omega_j \neq \omega'_j\}}.$$

To do so we use the Varshamov-Gilbert bound (cf. Lemma 5.1) that guarantees the existence of  $\Omega$  such that  $\text{card}(\Omega) \geq 2^{m/8}$  and  $\rho(\omega, \omega') \geq m/8$  for any  $\omega, \omega' \in \Omega$ . For such  $\Omega$  we have

$$d_\Delta(\Gamma_{p_\omega}, \Gamma_{p_{\omega'}}) \geq \frac{mq^{-d}}{4} \geq c_{40}q^{-\gamma\beta} \geq c_{41}n^{-\frac{\gamma\beta}{2\beta+d}}.$$

THIRD CONDITION:  $\max_{p, q \in \mathcal{N}} K(p, q) \leq c_{42} \log(s)$ .

Note that for the above choice of  $\Omega$ , we have  $s = \text{card}(\mathcal{N}) = \text{card}(\Omega) \geq 2^{m/8}$ . Therefore  $\log(s) \geq c_{43}m$  and we only have to prove that

$$\max_{p, q \in \mathcal{N}} K(p, q) \leq c_{44}m.$$

For any  $p_\omega, p_{\omega'} \in \mathcal{N}$ , we have,

$$\begin{aligned} K(p_\omega, p_{\omega'}) &= n \sum_{j \in \mathcal{J}} \int_{B_j \cup B_{j+1}} \log \left( \frac{1 + \omega_j \varphi_j(x)}{1 + \omega'_j \varphi_j(x)} \right) (1 + \omega_j \varphi_j(x)) dx \\ &\leq n \sum_{j \in \mathcal{J}} \int_{B_j \cup B_{j+1}} \log \left( \frac{1 + \omega_j \varphi_j(x)}{1 - \omega_j \varphi_j(x)} \right) (1 + \omega_j \varphi_j(x)) dx. \end{aligned}$$

Fix  $j \in \mathcal{J}$  and assume without loss of generality that  $\omega_j = 1$ . For any  $x \in B_j$  we have

$$\begin{aligned} \int_{B_j} \log \left( \frac{1 + \varphi_j(x)}{1 - \varphi_j(x)} \right) (1 + \varphi_j(x)) dx &= \\ &= \int_{B_j} \log \left( 1 + \frac{2\tilde{L}\|x - g_j\|_{\tilde{\beta}}^\beta}{1 - \tilde{L}\|x - g_j\|_{\tilde{\beta}}^\beta} \right) (1 + \tilde{L}\|x - g_j\|_{\tilde{\beta}}^\beta) dx \\ &= \int_{\mathcal{B}_{\tilde{\beta}}(0, \frac{1}{4q})} \log \left( 1 + \frac{2z(x)}{1 - z(x)} \right) (1 + z(x)) dx, \end{aligned}$$

where  $z(x) = \tilde{L}\|x\|_{\tilde{\beta}}^\beta$ . In the same manner, we have

$$\int_{B_{j+1}} \log \left( \frac{1 + \varphi_j(x)}{1 - \varphi_j(x)} \right) (1 + \varphi_j(x)) dx = \int_{\mathcal{B}_{\tilde{\beta}}(0, \frac{1}{4q})} \log \left( 1 - \frac{2z(x)}{1 + z(x)} \right) (1 - z(x)) dx.$$

Consider the function  $F : [0, 1) \rightarrow \mathbb{R}$  defined by

$$F(z) = \log \left( 1 + \frac{2z}{1 - z} \right) (1 + z) + \log \left( 1 - \frac{2z}{1 + z} \right) (1 - z).$$

For any  $z \geq 0$  such that  $z \leq \tilde{L}/4 \leq 1/4$ , we have

$$F(z) \leq \frac{2z(1+z)}{1-z} - \frac{2z(1-z)}{1+z} = \frac{8z^2}{1-z^2} \leq 9z^2.$$

It yields

$$\int_{B_j \cup B_{j+1}} \log \left( \frac{1 + \varphi_j(x)}{1 - \varphi_j(x)} \right) (1 + \varphi_j(x)) dx \leq 9 \int_{\mathcal{B}_{\tilde{\beta}}(0, \frac{1}{4q})} \|x\|_{\tilde{\beta}}^{2\beta} dx \leq c_{45} q^{(2\beta+d)}.$$

Hence

$$K(p_\omega, p_{\omega'}) \leq c_{45} n m q^{(2\beta+d)} \leq c_{46} m \leq c_{47} \log(s).$$

We can therefore apply Lemma 5.2 and the Theorem 4.1 is proved.  $\blacksquare$

## 5 Appendix

In this section we gather technical results that are used in Section 4. For a recent survey on the construction of minimax lower bounds, see Tsybakov

(2004a)[Chap. 2]. We first give a lemma related to subset extraction. Fix an integer  $m \geq 1$  and define

$$\Omega = \{\omega = (\omega_1, \dots, \omega_m), \omega_i \in \{0, 1\}\} = \{0, 1\}^m$$

For any two  $\omega = (\omega_1, \dots, \omega_m)$  and  $\omega' = (\omega'_1, \dots, \omega'_m)$  in  $\Omega$  define the *Hamming distance* between  $\omega$  and  $\omega'$  by

$$\rho(\omega, \omega') = \sum_{i=1}^m \mathbb{1}_{\{\omega_i \neq \omega'_i\}}.$$

The following lemma holds

**Lemma 5.1 (Varshamov-Gilbert bound, 1962)** *Fix  $m \geq 8$ . Then there exists a subset  $\{\omega^{(0)}, \dots, \omega^{(M)}\}$  of  $\Omega$  such that  $M \geq 2^{m/8}$  and*

$$\rho(\omega^{(j)}, \omega^{(k)}) \geq \frac{m}{8}, \quad \forall 0 \leq j < k \leq M.$$

Moreover, we can always take  $\omega^{(0)} = (0, \dots, 0)$ .

For a proof of this lemma, see Tsybakov (2004a, Lemma 2.8, p. 89).

The next lemma can be found in Tsybakov (1997, Lemma 4) and is stated here in a slightly weaker form. It allows to derive minimax lower bounds in the context of density level set estimation. It involves the Kullback-Leibler divergence between two probability densities  $p$  and  $q$  on  $\mathbb{R}^d$

$$K(p, q) = \begin{cases} \int_{\mathbb{R}^d} \log\left(\frac{p(x)}{q(x)}\right) p(x) dx & \text{if } P_p \ll P_q, \\ +\infty & \text{else.} \end{cases}$$

**Lemma 5.2** *Let  $d$  be a pseudo-metric between subsets of  $\mathcal{X} \subset \mathbb{R}^d$ . Let  $\mathcal{P}$  be a set of densities and assume that there exists a subset  $\mathcal{N} \subset \mathcal{F}$  with cardinal  $2 \leq \text{card}(\mathcal{N}) = s < \infty$  and a constant  $c_{48} > 0$ , such that*

$$d(\Gamma_p(\lambda), \Gamma_q(\lambda)) \geq \varepsilon, \quad \forall p, q \in \mathcal{N}, p \neq q, \quad (5.1)$$

and

$$\max_{p, q \in \mathcal{N}} K(p, q) \leq c_{48} \log(s), \quad (5.2)$$

where  $K(\cdot, \cdot)$  denotes the Kullback-Leibler divergence. Then, there exists an absolute positive constant  $c_{55}$  such that for any estimator  $\hat{G}_n$  of  $\Gamma_p(\lambda)$  constructed from the sample  $X_1, \dots, X_n$ , we have

$$\sup_{p \in \mathcal{P}} \mathbb{E} \left[ d(\Gamma_p(\lambda), \hat{G}_n) \right] \geq c_{49} \varepsilon.$$



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