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# Nonparametric estimation of regression level sets using kernel plug-in estimator

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## ABSTRACT

Let  $(X, Y)$  be a random pair taking values in  $\mathbb{R}^d \times J$ , where  $J \subset \mathbb{R}$  is supposed to be bounded. We propose a plug-in estimator of the level sets of the regression function  $r$  of  $Y$  on  $X$ , using a kernel estimator of  $r$ . We consider an error criterion defined by the volume of the symmetrical difference between the real and estimated level sets. We state the consistency of our estimator, and we get a rate of convergence equivalent to the one obtained by Cadre (2006) for the density function level sets.

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## 1. Introduction

In this paper, we consider the problem of estimating the level sets of a regression function. More precisely, consider a random pair  $(X, Y)$  taking values in  $\mathbb{R}^d \times J$ , where  $J \subset \mathbb{R}$  is supposed to be bounded. The goal of this paper is then to build an estimator of the level sets of the regression function  $r$  of  $Y$  on  $X$ , defined for all  $x \in \mathbb{R}^d$  by

$$r(x) = \mathbb{E}[Y|X = x].$$

For  $t > 0$ , a level set for  $r$  is defined by

$$\mathcal{L}(t) = \{x \in \mathbb{R}^d : r(x) > t\}.$$

Assume that we have an independent and identically distributed sample (i.i.d.)  $((X_1, Y_1), \dots, (X_n, Y_n))$  with the same distribution as  $(X, Y)$ . We then consider a plug-in estimator of  $\mathcal{L}(t)$ . More precisely, we use a consistent estimator  $\hat{r}_n$  of  $r$ , in order to estimate  $\mathcal{L}(t)$  by

$$\mathcal{L}_n(t) = \{x \in \mathbb{R}^d : \hat{r}_n(x) > t\}.$$

Most of the research works on the estimation of level sets concern the density function. One can cite the works of Cadre (2006), Cuevas and Fraiman (1997), Hartigan (1987), Polonik (1995), Tsybakov (1997), Walther (1997). This large number of works on this subject is motivated by the high number of possible applications. Estimating these level sets can be useful in mode estimation (Müller & Sawitzki, 1991; Polonik, 1995), or in clustering (Biau, Cadre, & Pelletier, 2007; Cuevas, Febrero, &

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Let  $K$  be a kernel on  $\mathbb{R}^d$ , that is a probability density on  $\mathbb{R}^d$ . We denote  $h = h_n$  and  $K_h(x) = K(x/h)$ . From an i.i.d. sample  $((X_1, Y_1), \dots, (X_n, Y_n))$ , we define, for all  $x \in \mathbb{R}^d$ ,

$$\varphi_n(x) = \frac{1}{nh^d} \sum_{i=1}^n Y_i K_h(x - X_i) \quad \text{and} \quad f_n(x) = \frac{1}{nh^d} \sum_{i=1}^n K_h(x - X_i).$$

For all  $x \in \mathbb{R}^d$ , the kernel estimator of  $r$  is then defined by

$$r_n(x) = \begin{cases} \varphi_n(x)/f_n(x) & \text{if } f_n(x) \neq 0 \\ 0 & \text{otherwise.} \end{cases}$$

The properties of this estimator are already well studied in the literature. For instance, the interesting reader can look at [Bosq and Lecoutre \(1987\)](#) or [Gasser and Müller \(1979\)](#).

Under the assumption

A0 There exists  $t^- < t$  such that  $\mathcal{L}(t^-)$  is compact. Besides,  $\lambda(\{r = t\}) = 0$  (where  $\lambda$  stands for the Lebesgue measure), a first consistency result can be trivially obtained from a slight modification of Theorem 3 by [Cuevas, González-Manteiga, and Rodríguez-Casal \(2006\)](#) and the consistency properties of the kernel estimator.

**Proposition 2.1.** *Under Assumption A0, if  $K$  is bounded, integrable, with compact support and Lipschitz, and if  $h \rightarrow 0$  and  $nh^d / \log n \rightarrow \infty$ , then*

$$\mathbb{E} \lambda(\mathcal{L}_n(t) \Delta \mathcal{L}(t)) \xrightarrow[n \rightarrow \infty]{} 0.$$

Note that the last part of assumption A0 means that the regression function cannot have a null derivative at the estimated level set.

### 2.2. Rate of convergence

From now on,  $\Theta \subset (0, \sup_{\mathbb{R}^d} r)$  is an open interval. Let us introduce the following assumptions:

A1 The functions  $r$  and  $f$  are twice continuously differentiable, and,  $\forall t \in \Theta, \exists 0 < t^- < t : \inf_{\mathcal{L}(t^-)} f > 0$ ;

A2 For all  $t \in \Theta$ ,

$$\inf_{r^{-1}(t)} \|\nabla r\| > 0,$$

where,  $\nabla \psi(x)$  stands for the gradient at  $x \in \mathbb{R}^d$  of the differentiable function  $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ .

The assumptions A1 on the regularity are inherited from the classical assumptions in kernel estimation ([Bosq & Lecoutre, 1987](#)). Note that “harder” assumptions on the regularity of  $r$  and  $f$  will not improve the obtained rate of consistency. Moreover, let us mention that under Assumptions A1 and A2, we have (Proposition A.2 in [Cadre \(2006\)](#))

$$\forall t \in \Theta : \lambda(r^{-1}[t - \varepsilon, t + \varepsilon]) \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0.$$

Let us now introduce the assumptions on the kernel  $K$ .

A3  $K$  is a continuously differentiable with a compact support. Moreover, there exists a decreasing function  $\mu : \mathbb{R}^+ \rightarrow \mathbb{R}$  such that  $K(x) = \mu(\|x\|)$  for all  $x \in \mathbb{R}^d$ .

We are now in a position to establish a rate of convergence for  $\mathbb{E} \lambda(\mathcal{L}_n(t) \Delta \mathcal{L}(t))$ .

**Theorem 2.1.** *Under Assumptions A0–A3, if  $nh^d / (\log n) \rightarrow \infty$  and  $nh^{d+4} \log n \rightarrow 0$ , then for almost all  $t \in \Theta$*

$$\mathbb{E} \lambda(\mathcal{L}_n(t) \Delta \mathcal{L}(t)) = O(1/\sqrt{nh^d}).$$

**Remarks.** • Roughly speaking, the assumptions about the bandwidth impose to take  $h$  between  $(\frac{\log n}{n})^{\frac{1}{d}}$  and  $(n \log n)^{\frac{-1}{d+4}}$ .

Moreover, if we take  $h = O((n \log n)^{\frac{-1}{d+4}})$ , we get

$$\begin{aligned} \sqrt{nh^d} &= O\left(\frac{n^{\frac{2}{d+4}}}{(\log n)^{\frac{d}{2(d+4)}}}\right) \\ &= O\left(\frac{n^{1/3}}{(\log n)^{1/6}}\right) \quad \text{with } d = 2, \end{aligned}$$

that is a rate of the same order as [Cadre \(2001\)](#) in the density case.

- A remaining and crucial problem is the research of an optimal bandwidth  $h$  for our estimator. Indeed, if they are already results in the literature about an optimal bandwidth for the estimation of  $r$ , this bandwidth is not necessarily optimal for estimating  $\mathcal{L}(t)$ . However, in the simulations, we used a cross-validation procedure to choose a bandwidth.



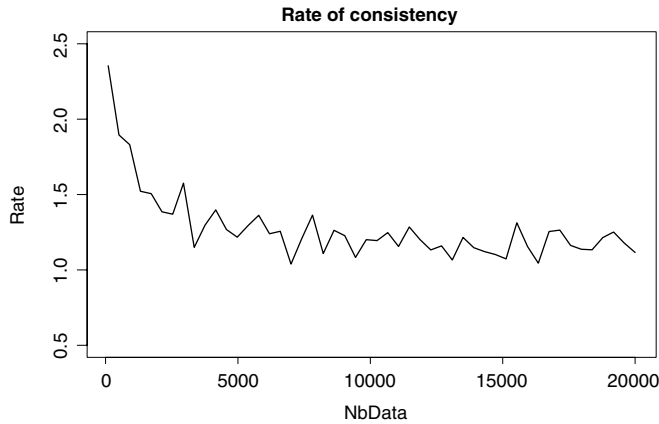


Fig. 3. Illustration of the rate: the curve represents the estimated error multiplied by  $\sqrt{nh^2}$ .

### 3.2. Selection of $h$ by cross-validation

Now we use a simple cross-validation to select the bandwidth: for each value of  $n$  we use half the dataset to compute the kernel estimator with  $h$  (and the level set estimator) on a grid of 20 values between the limits allowed by the assumptions of Theorem 2.1 (see the first remark below Theorem 2.1). Then, we use the remaining part of the dataset to evaluate the volume of the symmetrical difference and select the optimal  $h$ . We compare the error obtained to the previous ones in Fig. 4.

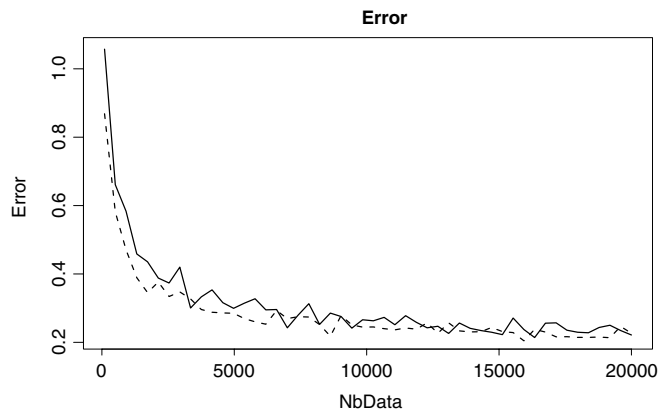


Fig. 4. Comparison of the error: the plain line stands for  $h = (n \log n)^{-1.1/6}$ , and the dotted line for  $h$  selected by a cross-validation.

We see that our choice process of  $h$  does not improve the estimation of the level sets. If we compare the error multiplied by  $\sqrt{nh^2}$  (Fig. 5), we see that we select a lower bandwidth.

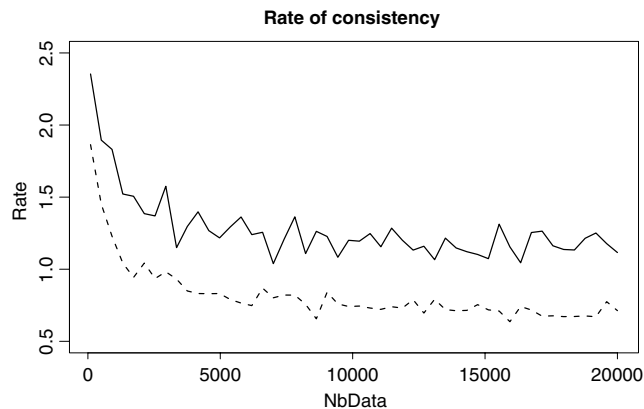


Fig. 5. Comparison of the rates: the plain line stands for  $h = (n \log n)^{-1.1/6}$ , and the dotted line for  $h$  selected by a cross-validation.

However, we cannot generalize about it since we are here in a very simple case. Moreover, we use a naive cross-validation method. Looking for more efficient methods to derive an optimal bandwidth for the level-set estimation is still an interesting and opened question. For this, we could first think of the adaptation of method used for density level set estimation like Rinaldo, Singh, Nugent, and Wasserman (2012) or Samworth and Wand (2010) for example.

4. Proofs

This section is dedicated to the proof of Theorem 2.1. From now on,  $c$  is a non-negative constant, which value may change from line to line.

4.1. Proof of Theorem 2.1

In this proof, some arguments are classical result from the kernel density (or regression) estimation theory. For more details, we refer the reader to the book by Bosq and Lecoutre (1987, Chapters 4 and 5).

From now on, we denote by  $\partial A$  the boundary of any subset  $A \subset \mathbb{R}^d$ . Besides, we introduce  $\mathcal{H}$  the  $(d - 1)$ -dimensional Hausdorff measure (Evans & Gariepy, 2000). Recall that  $\mathcal{H}$  agrees with ordinary “ $(k - 1)$ -dimensional surface area” on nice sets (Proposition A.1 in Cadre (2006)). Finally, we set  $\tilde{K} = \int K^2 d\lambda$ .

4.1.1. Preliminary results

All the results in this sections are stated under Assumptions A0–A3. The proof of the theorem relies on the four following lemmas.

Let us define

$$\Omega_{n,c} = \left\{ \sqrt{nh^d} \sup_{\mathcal{L}_n(t) \cup \mathcal{L}(t)} |r_n - r| \geq c\sqrt{\log n} \right\}.$$

**Lemma 4.1.** *If  $nh^{d+4}/\log n \rightarrow 0$ , then there exists  $\Gamma > 0$  such that*

$$\sqrt{nh^d} \mathbb{P}(\Omega_{n,\Gamma}) \rightarrow 0.$$

Note that the condition  $nh^{d+4}/\log n \rightarrow 0$  is satisfied under the assumptions of Theorem 2.1.

**Proof of Lemma 4.1.** As  $r$  is continuous, we have  $\sup_{\mathcal{L}(t^-)} |r| < c$ . Assuming that  $\inf_{\mathcal{L}(t^-)} f > 0$ , then, since  $\sup_{\mathcal{L}(t^-)} |f_n - f| \rightarrow 0$  a.s. under the assumptions of Lemma 4.1 (Bosq & Lecoutre, 1987), there exists  $\theta > 0$  such that  $\inf_{\mathcal{L}(t^-)} f_n > \theta$  a.s. for  $n$  large enough. So we can write

$$\begin{aligned} \sup_{\mathcal{L}(t^-)} |r_n - r| &= \sup_{\mathcal{L}(t^-)} \left| \frac{\varphi_n - \varphi}{f_n} + r \frac{f_n - f}{f_n} \right| \\ &\leq c \left( \sup_{\mathcal{L}(t^-)} |\varphi_n - \varphi| + \sup_{\mathcal{L}(t^-)} |f_n - f| \right). \end{aligned} \tag{1}$$

We have

$$\sup_{\mathcal{L}(t^-)} |\varphi_n - \varphi| \leq \sup_{\mathcal{L}(t^-)} |\varphi_n - \mathbb{E}\varphi_n| + \sup_{\mathcal{L}(t^-)} |\mathbb{E}\varphi_n - \varphi|.$$

We cover  $\mathcal{L}(t^-)$  with  $\ell_n$  balls  $B_k = B(x_k, \rho_n)$  ( $k = 1, \dots, \ell_n$ ) of radius  $\rho_n$ .

Consider  $x \in \mathcal{L}(t^-)$ , we denote by  $B_k$  the ball containing  $x$ . Then we set, for  $x, x' \in \mathcal{L}(t^-)$ ,

$$A_n(x, x') = \frac{1}{n} \sum_{i=1}^n Y_i [K_h(x - X_i) - K_h(x' - X_i)] - \mathbb{E} \frac{1}{n} \sum_{i=1}^n Y_i [K_h(x - X_i) - K_h(x' - X_i)],$$

which leads us to

$$\sup_{\mathcal{L}(t^-)} |\varphi_n - \varphi| \leq \sup_{1 \leq k \leq \ell_n} |\varphi_n(x_k) - \mathbb{E}\varphi_n(x_k)| + \sup_{x \in \mathcal{L}(t^-)} |A_n(x, x_k)| + \sup_{\mathcal{L}(t^-)} |\mathbb{E}\varphi_n - \varphi|. \tag{2}$$

Then, since  $K$  is Lipschitz, there exists  $\gamma > 0$  such that

$$\begin{aligned} |A_n(x, x_k)| &\leq ch^{-d-\gamma} \rho_n^\gamma \left( \frac{1}{n} \sum_{i=1}^n |Y_i| + \mathbb{E}|Y| \right) \\ &\leq ch^{-d-\gamma} \rho_n^\gamma \text{ since } Y \text{ is bounded.} \end{aligned}$$

As a consequence, we have

$$\mathbb{P} \left( \sup_{x \in \mathcal{L}(t^-)} |A_n(x, x_k)| > \frac{c}{4} \sqrt{\frac{\log n}{nh^d}} \right) \leq \mathbb{P} \left( ch^{-d-\gamma} \rho_n^\gamma > \frac{c}{4} \sqrt{\frac{\log n}{nh^d}} \right).$$

One can choose

$$\rho_n = n^{-a}, \quad a > 0 \quad \text{and} \quad \rho_n^\gamma = o \left( h^{d+\gamma} \sqrt{\frac{\log n}{nh^d}} \right),$$

such that

$$\mathbb{P} \left( \sup_{x \in \mathcal{L}(t^-)} |A_n(x, x_k)| > \log n / \sqrt{nh^d} \right) = 0. \tag{3}$$

Then, using the arguments of the proof of Theorem 5.II.3 in Bosq and Lecoutre (1987), we obtain

$$\forall \varepsilon > 0, \quad \mathbb{P} \left( \sup_{1 \leq k \leq l_n} |\varphi_n(x_k) - \mathbb{E}\varphi_n(x_k)| > \varepsilon \right) < 2\ell_n e^{-\frac{nh^d \varepsilon^2}{c}}.$$

If we set  $\varepsilon = \varepsilon_0 \sqrt{\log n / nh^d}$ , we have

$$\begin{aligned} \mathbb{P} \left( \sup_{1 \leq k \leq l_n} |\varphi_n(x_k) - \mathbb{E}\varphi_n(x_k)| > \varepsilon_0 \sqrt{\frac{\log n}{nh^d}} \right) &\leq c\ell_n n^{-2\varepsilon_0/c} \\ &\leq cn^{-2\varepsilon_0/c} \rho_n^{-d}. \end{aligned}$$

Remember that  $\rho_n = n^{-a}$ , with  $a > 0$ , one gets

$$\sqrt{nh^d} \mathbb{P} \left( \sup_{1 \leq k \leq l_n} |\varphi_n(x_k) - \mathbb{E}\varphi_n(x_k)| > \varepsilon_0 \sqrt{\frac{\log n}{nh^d}} \right) \leq cn^{1/2+ad-2\varepsilon_0/c} \sqrt{h^d} \tag{4}$$

which tends to 0 choosing  $\varepsilon_0 > \frac{(1/2+ad)c}{2}$ .

Moreover, under A3,  $K$  is even which gives us

$$\sup_{\mathcal{L}(t^-)} |\mathbb{E}\varphi_n - \varphi| = O \left( \sqrt{\frac{\log n}{nh^d}} \right),$$

and, using that  $nh^{d+4} / \log n \rightarrow 0$  we obtain

$$\sqrt{nh^d} \mathbb{P} \left( \sup_{\mathcal{L}(t^-)} |\mathbb{E}\varphi_n - \varphi| \geq \frac{c}{2} \sqrt{\frac{\log n}{nh^d}} \right) \rightarrow 0. \tag{5}$$

From (2) and using (3)–(5) we obtain

$$\sqrt{nh^d} \mathbb{P} \left( \sup_{\mathcal{L}(t^-)} |\varphi_n - \varphi| \geq c \sqrt{\frac{\log n}{nh^d}} \right) \rightarrow 0.$$

From (1) and such as  $\sup_{\mathcal{L}(t^-)} |f_n - f| \rightarrow 0$  a.s., we conclude the proof.  $\square$

Consider  $t \in \Theta$ . For all  $x \in \mathcal{L}(t^-)$ , we define

$$V_n(x, t) = \text{Var}((Y - t)K_h(x - X)) \quad \text{and} \quad \tilde{\mathbb{E}}r_n(x) = \mathbb{E}\varphi_n(x) / \mathbb{E}f_n(x).$$

For all  $x \in \mathcal{L}(t^-)$  such that  $V_n(x, t) \neq 0$ , we set

$$t_n(x) = \mathbb{E}f_n(x) \sqrt{\frac{nh^{2d}}{V_n(x, t)}} (t - \tilde{\mathbb{E}}r_n(x)).$$

Besides, we consider the sets

$$\mathcal{V}_n^t = r^{-1}[t, t + \Gamma \sqrt{\log n / nh^d}] \cap \mathcal{L}(t^-) \quad \text{and} \quad \tilde{\mathcal{V}}_n^t = r^{-1}[t - \Gamma \sqrt{\log n / nh^d}, t] \cap \mathcal{L}(t^-).$$

Finally, we denote by  $\Phi$  the distribution function of the standard normal  $\mathcal{N}(0, 1)$ , and we define  $\bar{\Phi}(x) = 1 - \Phi(x)$ .





**Proof of Lemma 4.4.** We only prove the first equation, the second one can be obtained with similar arguments.

Define  $E_n$  by

$$E_n = \sqrt{nh^d} \int_{\mathcal{V}_n^t} |\Phi(t_n(x))dx - \Phi(\bar{t}_n(x))dx|.$$

As  $\Phi$  is Lipschitz we have

$$E_n \leq c\sqrt{nh^d}\lambda(\mathcal{V}_n^t) \sup_{\mathcal{V}_n^t} |t_n - \bar{t}_n|. \tag{7}$$

By definition of  $t_n(x)$  and  $\bar{t}_n(x)$ , we have, for all  $x \in \mathcal{V}_n^t$ ,

$$\begin{aligned} \frac{1}{\sqrt{nh^d}} |t_n(x) - \bar{t}_n(x)| &\leq |t - r(x)| \left| \frac{f(x)}{\sqrt{\tilde{K}f(x)(v(x) + t^2)}} - \frac{\mathbb{E}f_n(x)}{\sqrt{V_n(x, t)h^{-d}}} \right| + \sqrt{\frac{h^d}{V_n(x, t)}} |\mathbb{E}f_n(x)r(x) - \tilde{\mathbb{E}}r_n(x)| \\ &\leq \sqrt{\frac{\log n}{nh^d}} \left| \sqrt{\frac{|f(x)V_n(x, t)h^{-d} - (\mathbb{E}f_n(x))^2\tilde{K}(v(x) + t^2)|}{\tilde{K}(v(x) + t^2)V_n(x, t)h^{-d}}} \right| \\ &\quad + \sqrt{\frac{h^d}{V_n(x, t)}} |\mathbb{E}f_n(x)r(x) - \tilde{\mathbb{E}}r_n(x)|. \end{aligned} \tag{8}$$

Remember that

$$|\tilde{\mathbb{E}}r_n(x) - r(x)| \leq \frac{1}{f_n(x)} |\mathbb{E}\phi_n(x) - \phi(x)| + |r(x)| |\mathbb{E}[f_n(x) - f(x)]|. \tag{9}$$

Since  $\mathcal{V}_n^t$  is included in  $\mathcal{L}(t^-)$ , we can deduce (Bosq & Lecoutre, 1987) from A1, A3 and (9) that

$$\sup_{x \in \mathcal{V}_n^t} |\tilde{\mathbb{E}}r_n(x) - r(x)| \leq ch^2. \tag{10}$$

Moreover, if we set

$$V_n^1(x) = \text{Var } K_h(x - X), \quad V_n^2 = \text{Var } Y K_h(x - X),$$

we can write

$$\begin{aligned} &|f(x)V_n(x, t)h^{-d} - (\mathbb{E}f_n(x))^2\tilde{K}(v(x) + t^2)| \\ &\leq |f(x)| |V_n(x, t)h^{-d} - \tilde{K}\mathbb{E}f_n(x)(v(x) + t^2)| + c|f(x) - \mathbb{E}f_n(x)| \\ &\leq |f(x)| |V_n(x, t)h^{-d} - \tilde{K}f(x)(v(x) + t^2)| + c|f(x) - \mathbb{E}f_n(x)| \\ &\leq |f(x)| (t^2|V_n^1(x)h^{-d} - \tilde{K}f(x)| + |V_n^2(x)h^{-d} - \tilde{K}f(x)v(x)| \\ &\quad + 2t |\text{Cov}(YK_h(x - X), K_h(x - X))|) + c|f(x) - \mathbb{E}f_n(x)| \\ &\leq c (|V_n^1(x)h^{-d} - \tilde{K}f(x)| + |V_n^2(x)h^{-d} - \tilde{K}f(x)v(x)| \\ &\quad + |\text{Cov}(YK_h(x - X), K_h(x - X))| + |f(x) - \mathbb{E}f_n(x)|). \end{aligned}$$

Again, since  $\mathcal{V}_n^t \subset \mathcal{L}(t^-)$ , we can deduce (Bosq & Lecoutre, 1987) from A1 and A3 that

$$\sup_{x \in \mathcal{V}_n^t} |f(x)V_n(x, t)h^{-d} - (\mathbb{E}f_n(x))^2\tilde{K}(v(x) + t^2)| \leq ch. \tag{11}$$

We deduce from (8), (10) and (11) that

$$\sup_{x \in \mathcal{V}_n^t} |t_n(x) - \bar{t}_n(x)| \leq c \left( \sqrt{h \log n} + \sqrt{nh^{k+4}} \right).$$

Then, thanks to (7) and since  $t \in \Theta_0$ , we have for  $n$  large enough

$$E_n \leq c\sqrt{\log n} \left( \sqrt{h \log n} + \sqrt{nh^{k+4}} \right), \tag{12}$$

which tends to 0 under the assumptions on  $h$  of Theorem 2.1. Finally, Lemma 4.2 leads us to

$$\sqrt{nh^d} \left[ \int_{\mathcal{V}_n^t} \mathbb{P}(r_n(x) < t)dx - \int_{\mathcal{V}_n^t} \Phi(t_n(x))dx \right] \leq c\lambda(\mathcal{V}_n^t)$$

which tends to 0 since  $\lambda(r^{-1}[t - \varepsilon, t + \varepsilon]) \rightarrow 0$ . This and (12) ends the proof.  $\square$



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