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Mathematical Properties of Continuous Ranked Probability Score Forecasting

Romain Pic^{a,*}, Clément Dombry^a, Philippe Naveau^b, Maxime Taillardat^{c,d}

^a Univ. Bourgogne Franche-Comté, CNRS UMR 6623, Laboratoire de Mathématiques de Besançon, 25000 Besançon, France

^b Laboratoire des Sciences du Climat et de l'Environnement, UMR 8212,

 $CEA/CNRS/UVSQ,\ EstimR,\ IPSL\ {\ensuremath{\mathcal E}}\ U\ Paris-Saclay,\ Gif-sur-Yvette,\ France$

^c CNRM, Université de Toulouse, Météo-France, CNRS, Toulouse, France ^d Météo-France, Toulouse, France

Abstract

The theoretical advances on the properties of scoring rules over the past decades have broaden the use of scoring rules in probabilistic forecasting. In meteorological forecasting, statistical postprocessing techniques are essential to improve the forecasts made by deterministic physical models. Numerous state-of-the-art statistical postprocessing techniques are based on distributional regression evaluated with the Continuous Ranked Probability Score (CRPS). However, the-oretical properties of such minimization of the CRPS have mostly considered the unconditional framework (i.e. without covariables) and infinite sample sizes. We circumvent these limitations and study the rate of convergence in terms of CRPS of distributional regression methods We find the optimal minimax rate of convergence for a given class of distributions. Moreover, we show that the k nearest neighbor method and the kernel method for the distributional regression reach the optimal rate of convergence in dimension $d \geq 2$ and in any dimension, respectively.

Keywords: Distributional Regression, Probabilistic Forecast, CRPS, Minimax Rate of Convergence, Nearest Neighbor Method, Kernel Method.

1 1. Introduction

In meteorology, ensemble forecasts are based on a given number of deterministic models whose parameters vary slightly in order to take into account observation errors and incomplete physical representation of the atmosphere. This leads to an ensemble of different forecasts that overall also assess the uncertainty of the forecast. Ensemble forecasts suffer from bias and underdispersion (Hamill & Colucci, 1997; Baran & Lerch, 2018) and need to be statistically postprocessed

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^{*}Corresponding author Email address: romain.pic@univ-fcomte.fr (Romain Pic)

in order to be improved. Different postprocessing methods have been proposed,
such as Ensemble Model Output Statistics (Gneiting et al., 2005), Quantile Regression Forests (Taillardat et al., 2019) or Neural Networks (Schulz & Lerch,
2021). These references, among other, also discuss the stakes of weather forecast
statistical postprocessing.

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Postprocessing methods rely on probabilistic forecast and distributional re-14 gression (Gneiting & Katzfuss, 2014) where the aim is to predict the conditional 15 distribution of the quantity of interest (e.g. temperatures, wind-speed, or pre-16 cipitation) given a set of covariates (e.g. ensemble model output statistics). 17 Algorithms are often based on the minimization of a proper scoring rule that 18 compares actual observations with the predictive distribution. Scoring rules 19 can be seen as an equivalent of a loss function in classical regression. A detailed 20 review of scoring rules is given by Gneiting & Raftery (2007). The Continu-21 ous Ranked Probability Score (CRPS; Matheson & Winkler, 1976), defined in 22 Equation (4), is one of the most popular score in meteorological forecasts. The 23 CRPS is also minimized to infer parameters of statistical models used in post-24 processing (e.g. Gneiting et al., 2005; Naveau et al., 2016; Rasp & Lerch, 2018; 25 Taillardat et al., 2019). 26

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To the best of our knowledge, most convergence statements about the CRPS are not only derived within an unconditional framework, i.e. without taking into account the covariates, but also these limiting results are based on infinite sample sizes. In this work, our goal is to bypass these two limitations. To go further, we need to set the stage by including a few notations.

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In this article, we consider the regression framework $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ with distribution P. In forecast assessment, we make the distinction between the construction of the estimator relying of the training sample $D_n = \{(X_i, Y_i), 1 \leq i \leq n\}$ and its evaluation with respect to new data (X, Y). Statistically, the goal of distributional regression is to estimate the conditional distribution of Y given X = x, noted $F_x^*(y)$: $= P(Y \leq y | X = x)$. Given the training sample D_n , the forecaster constructs a predictor $\hat{F}_n : x \mapsto \hat{F}_{n,x}$ that estimates the conditional distribution $F_x^*, x \in \mathbb{R}^d$. In this context, it is crucial to assess if $\hat{F}_{n,x}$ is close to F_x^* over the range of possible values of X = x. We denote by P_X the marginal distribution of X. The main goal of this work is to study the following positive quantity :

$$\mathbb{E}_{X \sim P_X, D_n \sim P^n} \left[\int_{\mathbb{R}} |\hat{F}_{n,X}(z) - F_X^*(z)|^2 \mathrm{d}z \right]$$
(1)

where $\mathbb{E}_{X \sim P_X, D_n \sim P^n}$ denotes the expectation with respect to X and D_n following P_X and P^n respectively. This averaged L^2 -norm is the distance between the predicted distribution $\hat{F}_{n,x}$ and the true conditional distribution F_x^* . We focus on this specific distance because it corresponds to the excess of risk associated with the CRPS, i.e. it is the difference between the expected CRPS for the predicted distribution $\hat{F}_{n,x}$ and the expected CRPS for the ideal prediction F_x^* , 40 see Section 2.1 for more details.

In order to study the rate of convergence of (1) as $n \to \infty$, we will adapt 42 the notion of optimal minimax rate of convergence that quantifies the best error 43 that an estimator can achieve uniformly on a given family of distributions \mathcal{D} 44 when the size of the training set D_n gets large. Stone (1982) provided minimax 45 rates of convergence within a point regression framework and the minimax the-46 ory for nonparametric regression is well-developed, see e.g. Györfi et al. (2002) 47 or Tsybakov (2009). To the extent of our knowledge, this paper states the first 48 results for distributional regression. 49

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Many predictors $\hat{F}_{n,x}$ can be studied and achieve the optimal minimax rate of convergence. To go further, we focus on two cases : k-nearest neighbor and kernel estimators.

The k-nearest neighbor (k-NN) method is well-known in the classical framework of regression and classification (see, e.g. Biau & Devroye, 2015). In distributional regression, the k-NN method can be suitably adapted to estimate the conditional distribution F_x^* and the estimator is written as

$$\hat{F}_{n,x}(z) = \frac{1}{k_n} \sum_{i=1}^{k_n} \mathbb{1}_{Y_{i:n}(x) \le z},$$
(2)

where $1 \leq k_n \leq n$ and $Y_{i:n}(x)$ denotes the observation at the *i*-th nearest neighbor of x. As usual, possible ties are broken at random to define nearest neighbors.

The kernel estimate in distributional regression (see, e.g. Chapter 5 of Györfi et al., 2002) can be expressed as

$$\hat{F}_{n,x}(z) = \frac{\sum_{i=1}^{n} K(\frac{x-X_i}{h_n}) \mathbb{1}_{Y_i \le z}}{\sum_{i=1}^{n} K(\frac{x-X_i}{h_n})},$$
(3)

if the denominator is nonzero. When the denominator is zero, we use the convention $\hat{F}_{n,x}(z) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{Y_i \leq z}$. Here the bandwidth $h_n > 0$ depends on the sample size n, and the function $K : \mathbb{R}^d \to [0, \infty)$ is called the kernel.

Minimax rates of convergence of the k-NN and kernel models in point re-58 gression are well-studied and it is known that, for suitable choices of number 59 of neighbors k_n and bandwidth h_n respectively, the methods are minimax rate 60 optimal on classes of distributions with Lipschitz or more generally Hölder con-61 tinuous regression functions (see e.g. Theorem 14.5 in Biau & Devroye, 2015 62 and Theorem 5.2 in Györfi et al., 2002). For classes of distributions where the 63 conditional distribution F_x^* satisfies some regularity requirements with respect to the covariates x (see Definition 1 of class $\mathcal{D}^{(h,C,M)}$), we are able to extend 64 65 these results to distributional regression. We obtain non asymptotic bounds for 66 the minimax rate of convergence for both the k-NN and kernel models. 67

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To summarize, this paper is organized as follows. Our main results are 69 presented in Section 2. Section 2.1 provides the theoretical background on 70 distributional regression and its evaluation using the CRPS. In Section 2.2, we 71 study the k-NN estimators (2) and derive a non asymptotic upper bound for the 72 excess of risk (1) uniformly on the class $\mathcal{D}^{(h,C,M)}$. Section 2.3 provides similar 73 results for the kernel method (3). In Section 2.4, we find a lower minimax rate 74 of convergence by reducing the problem to standard point regression solved by 75 Györfi et al. (2002). We can deduce that the k-NN method for the distributional 76 regression reaches the optimal rate of convergence in dimension d > 2, while the 77 kernel method reaches the optimal rate of convergence in any dimension. The 78 proofs of all the results presented in Section 2 are detailed in Appendix. 79

⁸⁰ 2. Main results

81 2.1. CRPS and distributional regression

The Continuous Ranked Probability Score (CRPS; Matheson & Winkler, 1976) compares a predictive distribution F and a real-valued observation y by computing the following integral

$$\operatorname{CRPS}(F, y) = \int_{\mathbb{R}} (F(z) - \mathbb{1}_{y \le z})^2 \mathrm{d}z.$$
(4)

The expected CRPS of a predictive distribution F when the observations Y are distributed according to G is defined as

$$\overline{\text{CRPS}}(F,G) = \int_{\mathbb{R}} \text{CRPS}(F,y)G(\mathrm{d}y), \quad F,G \in \mathcal{M}(\mathbb{R})$$
(5)

where $\mathcal{M}(\mathbb{R})$ denotes the set of all distribution functions on \mathbb{R} . This quantity is finite when both F and G have a finite moment of order 1. Then, the difference between the expected CRPS of the forecast F and the expected CRPS of the ideal forecast G can be written as

$$\overline{\text{CRPS}}(F,G) - \overline{\text{CRPS}}(G,G) = \int_{\mathbb{R}} |F(z) - G(z)|^2 dz \ge 0.$$
(6)

This implies that the only optimal prediction, in the sense that it minimizes the expected CRPS, is the true distribution G. A score with this property is said to be *strictly proper*. This property is essential for distributional regression as it justifies the minimization of the expected score in order to construct or evaluate a prediction.

Example 1. (CRPS for Generalized Pareto distributions)

Explicit parametric formulas of the CRPS exist for most classical distribution families : e.g. Gaussian, logistic, censored logistic, Generalized Extreme Value, Generalized Pareto (see Gneiting et al., 2005; Taillardat et al., 2016; Friederichs & Thorarinsdottir, 2012). We focus here on the Generalized Pareto Distribution

(GPD) family and we denote by $H_{\xi,\sigma}$ the GP distribution with shape parameter $\xi \in \mathbb{R}$ and scale parameter $\sigma > 0$. Recall that it is defined, when $\xi \neq 0$, by

$$H_{\xi,\sigma}(z) = 1 - \left(1 + \frac{\xi z}{\sigma}\right)_{+}^{-1/\xi}, \quad z > 0,$$

with the notation $(\cdot)_+ = \max(0, \cdot)$. When $\xi = 0$, the standard limit by continuity is used. For $\xi < 1$, the GPD has a finite first moment and the associated CRPS is given by (Friederichs & Thorarinsdottir, 2012)

$$\operatorname{CRPS}\left(H_{\xi,\sigma},y\right) = \left(y + \frac{\sigma}{\xi}\right)\left(2H_{\xi,\sigma}(y) - 1\right) - \frac{2\sigma}{\xi(\xi - 1)}\left(\frac{1}{\xi - 2} + \left(1 - H_{\xi,\sigma}(y)\right)\left(1 + \xi\frac{y}{\sigma}\right)\right)$$
(7)

When $Y \sim H_{\xi^*,\sigma^*}$, the expected CRPS is (Taillardat et al., 2022)

$$\overline{\text{CRPS}}(H_{\xi,\sigma}, H_{\xi^*,\sigma^*}) = \frac{\sigma^*}{1-\xi^*} + \frac{2\sigma}{1-\xi}m_0 + \frac{2\xi}{1-\xi}m_1 + 2\sigma^*\left(\frac{1}{1-\xi} - \frac{1}{2(2-\xi)}\right)$$
(8)

with

$$m_0 = \mathbb{E}_{Y \sim H_{\xi,\sigma}} \left[\left(1 + \frac{\xi}{\sigma} Y \right)^{-1/\xi} \right], \quad m_1 = \mathbb{E}_{Y \sim H_{\xi,\sigma}} \left[Y \left(1 + \frac{\xi}{\sigma} Y \right)^{-1/\xi} \right].$$

In particular,

$$\overline{\text{CRPS}}\left(H_{\xi^*,\sigma^*}, H_{\xi^*,\sigma^*}\right) = \frac{\sigma^*}{(2-\xi^*)(1-\xi^*)}$$

In distributional regression, a predictor $\hat{F}:x\mapsto \hat{F}_x$ is evaluated thanks to its expected risk

$$R_P(\hat{F}) = \mathbb{E}_{(X,Y)\sim P} \left[\text{CRPS}(\hat{F}_X, Y) \right]$$
$$= \mathbb{E}_{X\sim P_X} \left[\overline{\text{CRPS}}(\hat{F}_X, F_X^*) \right].$$

This quantity is important as many distributional regression methods try to minimize it in order to improve predictions. When Y is integrable, Equation (6) implies

$$R_P(\hat{F}) - R_P(F^*) = \mathbb{E}_{(X,Y)\sim P} \left[\operatorname{CRPS}(\hat{F}_X, Y) - \operatorname{CRPS}(F_X^*, Y) \right]$$
$$= \mathbb{E}_{X\sim P_X} \left[\int_{\mathbb{R}} \left| \hat{F}_X(z) - F_X^*(z) \right|^2 \mathrm{d}z \right] \ge 0.$$
(9)

We recall that Bayes risk is the minimal theoretical risk over all possible predictors and that Bayes predictor is a predictor achieving Bayes risk. Thus, Equation (9) implies that $R_P(F^*)$ is Bayes risk and that $R_P(\hat{F}) = R_P(F^*)$ if and only if $\hat{F}_x = F_x^* P_X$ -a.e. An introduction to the notions of theoretical risk, Bayes risk and excess of risk can be found in Section 2.4 of Hastie et al. (2001).

Example 2. (GPD regression)

We illustrate the above statement in the case of a Generalized Pareto regression model where Y given X = x follows a GPD with shape parameter $\xi^*(x)$ and scale parameter $\sigma^*(x)$. Then, it is possible to show that Bayes risk is equal to

$$R_P(F^*) = \int_{\mathbb{R}^d} \frac{\sigma^*(x)}{(2 - \xi^*(x))(1 - \xi^*(x))} P_X(\mathrm{d}x)$$

when $0 < \xi^*(x) < 1$ for all $x \in \mathbb{R}^d$. For a forecast in the GPD class, i.e. F_x is a GPD with shape parameter $\xi(x)$ and scale parameter $\sigma(x)$, then the risk $R_P(F)$ is equal to Bayes risk if and only if $\xi(x) = \xi^*(x)$ and $\sigma(x) = \sigma^*(x) P_X$ -a.e.

Finally, we consider the case of a predictor \hat{F}_n built on a training sample $D_n = \{(X_i, Y_i), 1 \leq i \leq n\}$, as presented in the introduction, to estimate the conditional distribution of Y given X. Then, (X, Y) denotes a new independent observation used to evaluate the performances of \hat{F}_n . The predictor has the expected CRPS

$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] = \mathbb{E}_{D_n \sim P^n, (X, Y) \sim P}[\operatorname{CRPS}(\hat{F}_{n, X}, Y)],$$

with expectation taken both with respect to the training sample D_n and test observation (X, Y). Once again, when Y is integrable, the expected risk has a unique minimum given by $R_P(F^*)$. The excess of risk becomes

$$\mathbb{E}_{D_n \sim P^n} \left[R_P(\hat{F}_n) \right] - R_P(F^*)$$

= $\mathbb{E}_{D_n \sim P^n, X \sim P_X} \left[\int_{\mathbb{R}} \left| \hat{F}_{n,X}(z) - F_X^*(z) \right|^2 \mathrm{d}z \right] \ge 0.$ (10)

For large sample sizes, one expects that the predictor correctly estimates the conditional distribution and that the excess of risk tends to zero. A genuine question is to investigate the rate of convergence of the excess of risk to zero as the sample size $n \to \infty$. The risk depends on the distribution of observations and we want the model to perform well on large classes of distributions. Hence, we consider the standard minimax approach, see for instance Györfi et al. (2002) for the standard cases of regression and classification.

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We consider the following classes of distributions.

Definition 1. For $h \in (0,1]$, C > 0 and M > 0, let $\mathcal{D}^{(h,C,M)}$ be the class of distributions P such that $F_x^*(y) = P(Y \le y | X = x)$ satisfies :

- 106 *i*) $X \in [0,1]^d P_X$ -a.s.;
- 107 *ii)* For all $x \in [0,1]^d$, $\int_{\mathbb{R}} F_x^*(z)(1-F_x^*(z)) dz \le M$;
- 108 *iii*) $||F_{x'}^* F_x^*||_{L^2} \le C ||x' x||^h$ for all $x, x' \in [0, 1]^d$.

Remark 1. In condition i, $[0, 1]^d$ could be replaced by any compact set of \mathbb{R}^d . Condition ii) requires that $\overline{\operatorname{CRPS}}(F_x^*, F_x^*)$ remains uniformly bounded by M, which is a condition on the dispersion of the distribution F_X^* since its implies that the absolute mean error (MAE) remains uniformly bounded. Condition iii) is a regularity statement of the conditional distribution in the space $L^2(\mathbb{R})$. Conditions i) - iii) in Definition 1 are very similar to the conditions considered in the point regression framework, see Theorem 5.2 in Györfi et al. (2002).

Example 3. In the GPD regression framework, condition *ii*) is equivalent to $\sigma^*(x) \leq M(2 - \xi^*(x))(1 - \xi^*(x))$ when $0 < \xi^*(x) < 1$, for all $x \in [0, 1]^d$. The regularity condition *iii*) holds with constants C and h as soon as $x \mapsto \xi^*(x)$ and $x \mapsto \sigma^*(x)$ are both h-Hölder. For example, the popular case were the shape parameter $\xi^*(x)$ and the scale parameter $\sigma^*(x)$ are assumed to be linearly dependent on x (i.e. $\xi^*(x) = \xi_0 + \alpha \cdot x$ and $\sigma^*(x) = \sigma_0 + \beta \cdot x$ with $\alpha, \beta \in \mathbb{R}^d$) is in a class of distributions of Definition 1.

In the following, we study the convergence rate of the excess of risk in order
to obtain the optimal minimax convergence rate. The reasoning is divided into
three steps:

- 1. We provide in Section 2.2 an explicit and nonasymptotic upper bound for the excess of risk of the k-nearest neighbor model uniformly on the class $\mathcal{D}^{(h,C,M)}$; the upper bound is then optimized with a suitable choice of k = k(n).
- 2. In Section 2.3, we obtain similar results for the kernel model.

3. We show in Section 2.4 that $a_n = n^{-\frac{2h}{2h+d}}$ is a lower minimax rate of convergence; the main argument is that it is enough to consider a binary model when both the observation Y and prediction \hat{F}_X take values in $\{0, L\}$; we deduce that in this case, the CRPS coincides with the mean squared error so that we can appeal to standard results on lower minimax rate of convergence for regression.

Combining these three steps, we finally obtain Theorem 1 providing the optimal minimax rate of convergence of the excess of risk on the class $\mathcal{D}^{(h,C,M)}$. All the proofs are postponed to the Appendix.

140 2.2. Upper bound for the k-nearest neighbor model

The k-NN method for distributional regression is defined in Equation (2). Here, we do not use only the mean of the nearest neighbor sample $(Y_{i:n}(x))_{1 \le i \le k_n}$ but its entire empirical distribution. Interestingly, the tools developed to analyze the k-NN in point regression can be used in our distributional regression framework.

Proposition 1. Assume $P \in \mathcal{D}^{(h,C,M)}$ and let \hat{F}_n be the k-nearest neighbor

model defined by Equation (2). Then,

$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*) \leq \begin{cases} 8^h C^2 \left(\frac{k_n}{n}\right)^h + \frac{M}{k_n} & \text{if } d = 1, \\ c_d^h C^2 \left(\frac{k_n}{n}\right)^{2h/d} + \frac{M}{k_n} & \text{if } d \ge 2, \end{cases}$$

where $c_d = \frac{2^{3+\frac{2}{d}}(1+\sqrt{d})^2}{V_d^{2/d}}$ and V_d is the volume of the unit ball in \mathbb{R}^d .

Let us stress that the upper bound is non-asymptotic and holds for all fixed n and k_n . Optimizing the upper bound in k_n yields the following corollary.

Corollary 1. Assume $P \in \mathcal{D}^{(h,C,M)}$ and consider the k-NN model (2).

• For
$$d = 1$$
, the optimal choice $k_n = \left(\frac{M}{hC^28^h}\right)^{\frac{1}{h+1}} n^{\frac{h}{h+1}}$ yields
$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*) \leq Bn^{-\frac{h}{h+1}}$$

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with constant
$$B = C^{\frac{2}{h+1}} M^{\frac{h}{h+1}} \left(8^{\frac{h}{h+1}} h^{-\frac{h}{h+1}} + (8^h h C)^{\frac{1}{h+1}}\right).$$

• For $d \ge 2$, the optimal choice $k_n = \left(\frac{Md}{2hC^2c_d^h}\right)^{\frac{d}{2h+d}} n^{\frac{2h}{2h+d}}$ yields

$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*) \le Bn^{-\frac{2h}{2h+d}}$$

with constant $B = (C^2 c_d^h)^{\frac{d}{2h+d}} M^{\frac{2h}{2h+d}} \left(\left(\frac{d}{2h}\right)^{\frac{2h}{2h+d}} + \left(\frac{2h}{d}\right)^{\frac{d}{2h+d}} \right).$

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153 2.3. Upper bound for the kernel model

Kernel methods adapted to distributional regression are defined in Equation (3). For convenience and simplicity of notations, we develop our result for the simple uniform kernel $K(x) = \mathbb{1}_{\{||x|| \le 1\}}$. However, it should be stressed that all the results can be extended to boxed kernels (Györfi et al., 2002, Figure 5.7 p73) to the price of some extra multiplicative constants. For the uniform kernel, the estimator writes

$$\hat{F}_{n,x}(z) = \frac{\sum_{i=1}^{n} \mathbb{1}_{\{\|X_i - x\| \le h_n\}} \mathbb{1}_{\{Y_i \le z\}}}{\sum_{i=1}^{n} \mathbb{1}_{\{\|X_i - x\| \le h_n\}}},$$
(11)

when the denominator is non zero and $\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{Y_i \leq z\}}$ otherwise.

Proposition 2. Assume $P \in \mathcal{D}^{(h,C,M)}$ and let \hat{F}_n be the kernel model defined by Equation (11). Then,

$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*) \le \tilde{c}_d \frac{2M + Cd^{h/2} + \frac{M}{n}}{nh_n^d} + C^2 h_n^{2h}$$

155 where \tilde{c}_d only depends on d.

Once again, the upper bound is non-asymptotic and holds for all fixed n and h_n . Optimizing the upper bound in h_n yields the following corollary.

Corollary 2. Assume $P \in \mathcal{D}^{(h,C,M)}$ and consider the kernel model (11). For any d, the optimal choice

$$h_n = \left(\frac{\tilde{c}_d d(M + Cd^{h/2} + \frac{M}{n})}{2hC^2}\right)^{\frac{1}{2h+d}} n^{-\frac{1}{2h+d}}$$

yields

$$\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*) \le Bn^{-\frac{2h}{2h+d}}$$

with

$$B = C^{\frac{2d}{2h+d}} \left(\tilde{c}_d (2M + Cd^{h/2} + \frac{M}{n}) \right)^{\frac{2h}{2h+d}} \left(\left(\frac{d}{2h} \right)^{-\frac{d}{2h+d}} + \left(\frac{d}{2h} \right)^{\frac{2h}{2h+d}} \right).$$

158 2.4. Optimal minimax rates of convergence

We finally compare the rates of convergence obtained in Corollaries 1 and 2 with a lower minimax rate of convergence in order to see whether the optimal rate of convergence are achieved. We first recall these different notions of minimax rates of convergence.

Definition 2. A sequence of positive numbers (a_n) is called an optimal minimax rate of convergence on the class \mathcal{D} if

$$\liminf_{n \to \infty} \inf_{\hat{F}_n} \sup_{P \in \mathcal{D}} \frac{\mathbb{E}_{D_n \sim P^n}[R_P(\hat{F}_n)] - R_P(F^*)}{a_n} > 0$$
(12)

and

$$\limsup_{n \to \infty} \inf_{\hat{F}_n} \sup_{P \in \mathcal{D}} \frac{\mathbb{E}_{D_n \sim P^n} [R_P(\hat{F}_n)] - R_P(F^*)}{a_n} < \infty,$$
(13)

where the infimum is taken over all distributional regression models \hat{F}_n trained on D_n . If the sequence (a_n) satisfies only the lower bound (12), it is called a lower minimax rate of convergence. To prove a lower bound on a class \mathcal{D} , it is always possible to consider a smaller class \mathcal{B} . Indeed, if $\mathcal{B} \subset \mathcal{D}$, we clearly have

$$\inf_{\hat{F}_n} \sup_{P \in \mathcal{B}} \left\{ \mathbb{E}_{D_n \sim P^n} [R_P(\hat{F}_n)] - R_P(F^*) \right\} \leq \inf_{\hat{F}_n} \sup_{P \in \mathcal{D}} \left\{ \mathbb{E}_{D_n \sim P^n} [R_P(\hat{F}_n)] - R_P(F^*) \right\}$$

so that any lower minimax rate of convergence on \mathcal{B} is also a lower minimax rate of convergence on \mathcal{D} .

To establish the lower minimax rate of convergence, we focus on the following classes of binary responses.

170 Definition 3.

171 Let $\mathcal{B}^{(h,C,L)}$ be the class of distributions of (X,Y) such that :

- i) $Y \in \{0, L\}$ and X is uniformly distributed on $[0, 1]^d$;
- 173 *ii)* $||F_{x'}^* F_x^*||_{L^2} \le C ||x' x||^h$ for all $x, x' \in [0, 1]^d$.

Since a binary outcome $Y \in \{0, L\}$ satisfies $\int_{\mathbb{R}} F_x^*(z)(1 - F_x^*(z))dz \leq L/4$, condition *ii*) in Definition 1 holds with $M \geq L/4$. Then $\mathcal{B}^{(h,C,L)} \subset \mathcal{D}^{(h,C,M)}$ and the following lower bound established on the smaller class also holds on the larger class.

Proposition 3. The sequence $a_n = n^{-\frac{2h}{2h+d}}$ is a lower minimax rate of convergence on the class $\mathcal{B}^{(h,C,L)}$. More precisely,

$$\liminf_{n \to \infty} \inf_{\hat{F}_n} \sup_{P \in \mathcal{B}^{(h,C,L)}} \frac{\mathbb{E}_{D_n \sim P^n}[R_P(F_n)] - R_P(F^*)}{C^{\frac{2d}{2h+d}}n^{-\frac{2h}{2h+d}}} \ge C_1 \tag{14}$$

for some constant $C_1 > 0$ independent of C.

Combining Corollaries 1 and 2 and Proposition 3, we can deduce that for $d \geq 2$, the k-NN model reaches the minimax lower rate of convergence $a_n = n^{-\frac{2h}{2h+d}}$ for the class $\mathcal{D}^{(h,C,M)}$ and that the kernel model reaches the minimax lower rate of convergence in any dimension d. This shows that the lower rate of convergence is in fact the optimal rate of convergence and proves the following theorem.

Theorem 1. The sequence $a_n = n^{-\frac{2h}{2h+d}}$ is the optimal minimax rate of convergence on the class $\mathcal{D}^{(h,C,M)}$.

It should be stressed that the rate of convergence $n^{-\frac{2h}{2h+d}}$ is the same as in point regression with square error, see Theorems 3.2 and 5.2 in Györfi et al. (2002) for the lower bound and upper bound, respectively.

¹⁹⁰ 3. Conclusion and Discussion

We found that the optimal rate of convergence for distributional regression on $\mathcal{D}^{(h,C,M)}$ is of the same order as the optimal rate of convergence for point regression. Thus, with regard to the sample size n, distributional regression evaluated with the CRPS converges at the same rate as point regression even though the distributional estimate carries more information on the prediction of the underlying process.

We have also shown that the k-NN method and the kernel method reach 197 this optimal rate of convergence, respectively in dimension d > 2 and in any 198 dimension. However, these methods are not used in practice because of the 199 limitations of their predictive power in moderate or high dimension $d \geq 3$ due 200 to the curse of dimension. An extension of this work could be to study if state-of-201 the-art techniques reach the optimal rate of convergence obtained in this article. 202 Random Forests (Breiman, 2001) methods, such as Quantile Regression Forests 203 (Meinshausen, 2006) and Distributional Random Forests (Cevid et al., 2020), 204 appear to be natural candidates as they are based on a generalized notion of 205 neighborhood and have been subject to recent development in weather forecast 206 statistical postprocessing (see, e.g., Taillardat et al., 2016). 207

The results of this article were obtained for the CRPS, which is widely used in practice, but can easily be extended to the weighted CRPS in its standard uses. The weighted CRPS is defined as

wCRPS
$$(F, y) = \int_{\mathbb{R}} (F(z) - \mathbb{1}_{y \le z})^2 w(z) dz$$

with w the weight chosen. The weighted CRPS is used to put the focus of the score in specific regions of the outcome space (Gneiting & Ranjan, 2011). It is used in the study of extreme events by giving more weight to the extreme behavior of the distribution.

Moreover, an interesting development would be to obtain similar results for rate of convergence with respect to different strictly proper scoring rules or metrics, for instance energy scores or Wasserstein distances.

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288 Appendix A. Proof of Proposition 1

For the simplicity of notation, we write simply \mathbb{E} for the expectation with respect to $(X, Y) \sim P$ and $D_n \sim P^n$. The context makes it clear enough so as to avoid confusion.

Proof. Recall that for the CRPS, the excess of risk is equal to

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) = \mathbb{E}\left[\int_{\mathbb{R}} |\hat{F}_{n,X}(z) - F_X^*(z)|^2 \mathrm{d}z\right].$$
 (A.1)

We first estimate $\mathbb{E}[|\hat{F}_{n,x}(z) - F_x^*(z)|^2]$ for fixed $x \in [0,1]^d$ and $z \in \mathbb{R}$. Denote by $X_{1:n}(x), \dots, X_{k_n:n}(x)$ the nearest neighbors of x and by $Y_{1:n}(x), \dots, Y_{k_n:n}(x)$ the associated values of the response variable. Conditionally on $X_{i:n}(x) = x_i$, $1 \leq i \leq k_n$, the random variables $Y_{i:n}(x), 1 \leq i \leq k_n$, are independent and with distribution $F_{x_i}^*$, $1 \leq i \leq k_n$. This implies that, conditionally, $\hat{F}_{n,x}(z)$ is the average of the k_n independent random variables $\mathbb{1}_{\{Y_{i:n}(x) \leq z\}}$ that have a Bernoulli distribution with parameter $F_{x_i}^*(z)$. Therefore, the conditional bias

and variance are given by

$$\mathbb{E}[\hat{F}_{n,x}(z) - F_x^*(z) \mid X_i(x) = x_i, 1 \le i \le k_n] = \frac{1}{k_n} \sum_{i=1}^{k_n} \left(F_{x_i}^*(z) - F_x^*(z) \right)$$
$$\operatorname{Var}[\hat{F}_{n,x}(z) \mid X_i(x) = x_i, 1 \le i \le k_n] = \frac{1}{k_n^2} \sum_{i=1}^{k_n} F_{x_i}^*(z)(1 - F_{x_i}^*(z)).$$

Adding up the squared conditional bias and variance and integrating with respect to $X_{i:n}(x)$, $1 \le i \le k_n$, we obtain the mean squared error

$$\mathbb{E}\left[|\hat{F}_{n,x}(z) - F_x^*(z)|^2\right] \\ = \mathbb{E}\left[\left(\frac{1}{k_n}\sum_{i=1}^{k_n} \left(F_{X_{i:n}(x)}^*(z) - F_x^*(z)\right)\right)^2\right] + \frac{1}{k_n^2}\sum_{i=1}^{k_n} \mathbb{E}\left[F_{X_{i:n}(x)}^*(z)(1 - F_{X_{i:n}(x)}^*(z))\right].$$

Using Jensen's inequality and integrating with respect to $P_X(dx)dz$, we deduce that the excess of risk (A.1) satisfies

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) \le \frac{1}{k_n} \sum_{i=1}^{k_n} \mathbb{E}\left[\int_{\mathbb{R}} (F^*_{X_{i:n}(X)}(z) - F^*_X(z))^2 \mathrm{d}z\right] \\ + \frac{1}{k_n^2} \sum_{i=1}^{k_n} \mathbb{E}\left[\int_{\mathbb{R}} F^*_{X_{i:n}(X)}(z)(1 - F^*_{X_{i:n}(X)}) \mathrm{d}z\right].$$

Using conditions ii) and iii) in the definition of the class $\mathcal{D}^{(h,C,M)}$ to bound from above the first and second term respectively, we get

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) \le \frac{C^2}{k_n} \sum_{i=1}^{k_n} \mathbb{E}[\|X_{i:n}(X) - X\|^{2h}] + \frac{M}{k_n}$$
$$\le C^2 \mathbb{E}[\|X_{k_n:n}(X) - X\|^{2h}] + \frac{M}{k_n},$$

where the last inequality uses the fact that, by definition of nearest neighbors, 292 293

the distances $||X_{i:n}(X) - X||$, $1 \le i \le k_n$, are non-increasing.

The last step of the proof is to use Theorem 2.4 from Biau & Devroye (2015) stating that

$$\mathbb{E}[\|X_{k_n:n}(X) - X\|^2] \le \begin{cases} 8\frac{k_n}{n} & \text{if } d = 1, \\ c_d \left(\frac{k_n}{n}\right)^{2/d} & \text{if } d \ge 2. \end{cases}$$

Together with the concavity inequality (as $h \in (0, 1]$)

$$\mathbb{E}[\|X_{k_n:n}(X) - X\|^{2h}] \le \mathbb{E}[\|X_{k_n:n}(X) - X\|^2]^h,$$

we deduce

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) \le \begin{cases} C^2 8^h \left(\frac{k_n}{n}\right)^h + \frac{M}{k_n} & \text{if } d = 1, \\ C^2 c_d^h \left(\frac{k_n}{n}\right)^{2h/d} + \frac{M}{k_n} & \text{if } d \ge 2, \end{cases}$$

concluding the proof of Proposition 1. 294

Appendix B. Proof of Proposition 2 295

Proof. Equation (11) can be rewritten as

$$\hat{F}_{n,x}(z) = \frac{\sum_{i=1}^{n} \mathbb{1}_{\{X_i \in S_{x,h_n}\}} \mathbb{1}_{\{Y_i \le z\}}}{n P_n(S_{x,h_n})},$$

with $S_{x,\epsilon}$ the closed ball centered at x of radius $\epsilon > 0$ and

$$P_n(\cdot) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \in \cdot\}}$$

the empirical measure corresponding to X_1, \ldots, X_n . Recall that we use the estimator $\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{Y_i \leq z\}}$ when $nP_n(S_{x,h_n}) = 0$. Similarly as in the proof of the Proposition 1, a bias/variance decomposition

of the squared error yields

$$\begin{split} & \mathbb{E}\left[|\hat{F}_{n,x}(z) - F_{x}^{*}(z)|^{2}\right] \\ &= \mathbb{E}\left[\left(\frac{\sum_{i=1}^{n}\left(F_{X_{i}(x)}^{*}(z) - F_{x}^{*}(z)\right)\mathbb{1}_{\{X_{i}\in S_{x,h_{n}}\}}}{nP_{n}(S_{x,h_{n}})}\right)^{2}\mathbb{1}_{\{nP_{n}(S_{x,h_{n}})>0\}} \right] \\ &+ \mathbb{E}\left[\frac{\sum_{i=1}^{n}F_{X_{i}}^{*}(z)(1 - F_{X_{i}}^{*}(z))\mathbb{1}_{\{X_{i}\in S_{x,h_{n}}\}}}{(nP_{n}(S_{x,h_{n}}))^{2}}\mathbb{1}_{\{nP_{n}(S_{x,h_{n}})>0\}}\right] \\ &+ \mathbb{E}\left[\left(\frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{\{Y_{i}\leq z\}} - F_{x}^{*}(z)\right)^{2}\mathbb{1}_{\{nP_{n}(S_{x,h_{n}})=0\}}\right] \\ &:= A_{1}(z) + A_{2}(z) + A_{3}(z). \end{split}$$

The excess of risk at X = x is thus decomposed into three terms

$$\mathbb{E}\left[\int_{\mathbb{R}} |\hat{F}_{n,x}(z) - F_x^*(z)|^2 \mathrm{d}z\right] = \int_{\mathbb{R}} A_1(z) \mathrm{d}z + \int_{\mathbb{R}} A_2(z) \mathrm{d}z + \int_{\mathbb{R}} A_3(z) \mathrm{d}z$$

that we analyze successively. 298

The first term (bias) is bounded from above using Jensen's inequality and property *iii*) of $\mathcal{D}^{(h,C,M)}$:

$$\begin{split} \int_{\mathbb{R}} A_{1}(z) \mathrm{d}z &\leq \mathbb{E} \left[\frac{\sum_{i=1}^{n} \int_{\mathbb{R}} \left(F_{X_{i}(x)}^{*}(z) - F_{x}^{*}(z) \right)^{2} \mathrm{d}z \mathbb{1}_{\{X_{i} \in S_{x,h_{n}}\}}}{n P_{n}(S_{x,h_{n}})} \mathbb{1}_{\{n P_{n}(S_{x,h_{n}}) > 0\}} \right] \\ &\leq \mathbb{E} \left[\frac{\sum_{i=1}^{n} C^{2} \|X_{i} - x\|^{2h} \mathbb{1}_{\{X_{i} \in S_{x,h_{n}}\}}}{n P_{n}(S_{x,h_{n}})} \mathbb{1}_{\{n P_{n}(S_{x,h_{n}}) > 0\}} \right] \\ &\leq C^{2} h_{n}^{2h}. \end{split}$$

The second term (variance) is bounded using property ii) of $\mathcal{D}^{(h,C,M)}$ and an elementary result for the binomial distribution:

$$\begin{split} \int_{\mathbb{R}} A_2(z) \mathrm{d}z &= \mathbb{E}\left[\frac{\sum_{i=1}^n \int_{\mathbb{R}} F_{X_i}^*(z)(1 - F_{X_i}^*(z)) \mathrm{d}z \mathbb{1}_{\{X_i \in S_{x,h_n}\}}}{(nP_n(S_{x,h_n}))^2} \mathbb{1}_{\{nP_n(S_{x,h_n}) > 0\}}\right] \\ &\leq M \mathbb{E}\left[\frac{\mathbb{1}_{\{nP_n(S_{x,h_n}) > 0\}}}{nP_n(S_{x,h_n})}\right] \\ &\leq \frac{2M}{nP_X(S_{x,h_n})}. \end{split}$$

In the last line, we use that $Z = nP_n(S_{x,h_n})$ follows a binomial distribution with parameters n and $p = P_X(S_{x,h_n})$ so that $\mathbb{E}\left[\frac{1}{Z}\mathbb{1}_{\{Z>0\}}\right] \leq \frac{2}{(n+1)p}$, see Lemma 4.1 in Györfi et al. (2002).

The last term is a remainder term and is bounded by

$$\int_{\mathbb{R}} A_{3}(z) dz \leq \mathbb{E} \left[\frac{1}{n} \int_{\mathbb{R}} \sum_{i=1}^{n} \left(F_{X_{i}}^{*}(z) - F_{x}^{*}(z) \right)^{2} dz \mathbb{1}_{\{nP_{n}(S_{x,h_{n}})=0\}} \right] \\ + \mathbb{E} \left[\frac{1}{n^{2}} \sum_{i=1}^{n} \int_{\mathbb{R}} F_{X_{i}}^{*}(z) (1 - F_{X_{i}}^{*}(z)) dz \mathbb{1}_{\{nP_{n}(S_{x,h_{n}})=0\}} \right].$$

Properties *ii*) and *iii*) of $\mathcal{D}^{(h,C,M)}$ and the fact that $||X_i - x|| \leq \sqrt{d}$ imply

$$\int_{\mathbb{R}} A_3(z) \mathrm{d}z \leq \left(Cd^{h/2} + \frac{M}{n} \right) \mathbb{E} \left[\mathbbm{1}_{\{nP_n(S_{x,h_n})=0\}} \right]$$
$$\leq \left(Cd^{h/2} + \frac{M}{n} \right) e^{-nP_X(S_{x,h_n})}.$$

For the second inequality, we use that $\mathbb{P}(Z = 0) = (1 - p)^n \leq e^{-np}$ where $Z = nP_n(S_{x,h_n})$ follows a binomial distribution with parameters n and $p = P_X(S_{x,h_n})$.

Collecting the three terms, we obtain the following upper bound for the excess of risk at X = x:

$$\mathbb{E}\left[\int_{\mathbb{R}} |\hat{F}_{n,x}(z) - F_x^*(z)|^2 \mathrm{d}z\right] \le C^2 h_n^{2h} + \frac{2M}{nP_X(S_{x,h_n})} + \left(Cd^{h/2} + \frac{M}{n}\right)e^{-nP_X(S_{x,h_n})}$$

We finally integrate this bound with respect to $P_X(dx)$. According to Equation (5.1) in Györfi et al. (2002), there exists a constant \tilde{c}_d depending only on d such that

$$\int_{[0,1]^d} \frac{1}{n P_X(S_{x,h_n})} P_X(\mathrm{d}x) \le \frac{\tilde{c}_d}{n h_n^d}$$

Note that \tilde{c}_d can be chosen as $\tilde{c}_d = d^{d/2}$. We also have

$$\int_{[0,1]^d} e^{-nP_X(S_{x,h_n})} P_X(\mathrm{d}x) \le \max_{u\ge 0} u e^{-u} \int_{[0,1]^d} \frac{1}{nP_X(S_{x,h_n})} P_X(\mathrm{d}x) \le \frac{\tilde{c}_d}{nh_n^d}.$$

We obtain thus

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) = \mathbb{E}\left[\int_{\mathbb{R}} |\hat{F}_{n,x}(z) - F_x^*(z)|^2 \mathrm{d}z\right]$$
$$\leq C^2 h_n^{2h} + \tilde{c}_d \frac{2M + Cd^{h/2} + \frac{M}{n}}{nh_n^d}.$$

305

306 Appendix C. Proof of Proposition 3

The proof of Proposition 3 relies on the next two elementary lemmas. The first one states that for a binary outcome $Y \in \{0, L\}$, forecasters should focus on binary forecast $F \in \mathcal{M}(\{0, L\})$ only, which is very natural. More precisely, any predictive distribution $F \in \mathcal{M}(\mathbb{R})$ can be associated with $F \in \mathcal{M}(\{0, L\})$ with a better expected CRPS.

Lemma 1. Let $G \in \mathcal{M}(\{0, L\})$. For $F \in \mathcal{M}(\mathbb{R})$, the distribution

$$\tilde{F}(z) = (1-m)\mathbb{1}_{0 \le z} + m\mathbb{1}_{L \le z}$$
 with $m = \frac{1}{L} \int_0^L (1-F(z)) dz$

satisfies

$$\overline{\mathrm{CRPS}}(\tilde{F}, G) \le \overline{\mathrm{CRPS}}(F, G).$$

Proof. Let $F \in \mathcal{M}(\mathbb{R})$ and $G \in \mathcal{M}(\{0, L\})$. We have

$$\overline{\text{CRPS}}(F,G) = \int_{\mathbb{R}} \int_{\mathbb{R}} (F(z) - \mathbb{1}_{y \le z})^2 dz G(dy)$$
$$\geq \int_{\mathbb{R}} \int_0^L (F(z) - \mathbb{1}_{y \le z})^2 dz G(dy)$$

Because 1 - m is the mean value of F on [0, L], we have for $y \in \{0, L\}$

$$\int_0^L (F(z) - \mathbb{1}_{y \le z})^2 \mathrm{d}z \ge \int_0^L ((1-m) - \mathbb{1}_{y \le z})^2 \mathrm{d}z.$$

Integrating with respect to G(dy), we deduce

$$\overline{\operatorname{CRPS}}(F,G) \ge \int_{\mathbb{R}} \int_0^L ((1-m) - \mathbb{1}_{y \le z})^2 \mathrm{d}z G(\mathrm{d}y).$$

The right hand side equals $\overline{\text{CRPS}}(\tilde{F}, G)$ and we conclude

$$\overline{\operatorname{CRPS}}(F,G) \ge \overline{\operatorname{CRPS}}(F,G).$$

31 2

Lemma 2 shows that for binary outcome and predictions, the CRPS reduces to a quantity proportional to the Brier score (Brier, 1950)

Brier
$$(p, y) = (y - p)^2, y \in \{0, 1\}, p \in [0, 1],$$

313 which is closely related to the mean squared error used in regression.

Lemma 2. For all $y \in \{0, L\}$ and $F(z) = (1-p)\mathbb{1}_{0 \le z} + p\mathbb{1}_{L \le z} \in \mathcal{M}(\{0, L\})$ with $p \in [0, 1]$, it holds

$$\operatorname{CRPS}(F, y) = L\operatorname{Brier}(p, \frac{y}{L}) = L(\frac{y}{L} - p)^2.$$

Proof. We compute

$$CRPS(F, y) = \int_0^L (1 - p - \mathbb{1}_{y \le z})^2 dz$$
$$= \begin{cases} Lp^2 & \text{if } y=0\\ L(1-p)^2 & \text{if } y=L \end{cases}.$$

In both cases, this equals $L(\frac{y}{L}-p)^2 = LBrier(p, \frac{y}{L})$.

Proof of Proposition 3. Since only binary outcomes are considered in the class $\mathcal{B}^{(h,C,L)}$, Lemma 1 implies that

$$\inf_{\hat{F}_n} \sup_{P \in \mathcal{B}^{(h,C,L)}} \left\{ \mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) \right\} = \inf_{\tilde{F}_n} \sup_{P \in \mathcal{B}^{(h,C,L)}} \left\{ \mathbb{E}[R_P(\tilde{F}_n)] - R_P(F^*) \right\}$$

where the infimum are taken over models \hat{F}_n and \hat{F}_n trained on the first observations $(X_i, Y_i)_{1 \le i \le n}$ and with values in $\mathcal{M}(\mathbb{R})$ and $\mathcal{M}(\{0, L\})$, respectively. Indeed, the left hand side is a priori smaller since the family \hat{F}_n is larger but Lemma 1 ensures that each model \hat{F}_n can be associated with a model \tilde{F}_n with equal or lower expected score.

We then apply Lemma 2. For a binary outcome, the conditional distribution of Y given X = x writes

$$F_x^*(z) = (1 - m(x)) \mathbb{1}_{0 \le z} + m(x) \mathbb{1}_{L \le z},$$

and the model \tilde{F}_n with values in $\mathcal{M}(\{0, L\})$ takes the form

$$F_{n,x}(z) = (1 - m_n(x)) \mathbb{1}_{0 \le z} + m_n(x) \mathbb{1}_{L \le z}$$

with $m(x) = \frac{1}{L} \int_0^L (1 - F_x^*(z)) dz$ and $m_n(x) = \frac{1}{L} \int_0^L (1 - \hat{F}_{n,x}(z)) dz$. Then Lemma 2 implies

$$\mathbb{E}[R_P(\hat{F}_n)] - R_P(F^*) = \mathbb{E}\left[\operatorname{CRPS}(\hat{F}_{n,X}, Y) - \operatorname{CRPS}(F_X^*, Y)\right]$$
$$= L\mathbb{E}\left[(Y/L - m_n(X))^2 - (Y/L - m(X))^2\right]$$
$$= L\mathbb{E}\left[(m_n(X) - m(X))^2\right],$$

which corresponds to the excess of risk in regression with squared error loss. The property iii) of $\mathcal{B}^{(h,C,L)}$ is equivalent to

$$|m(x) - m(x')|^h \le C ||x - x'||^h, \quad x \in [0, 1]^d,$$

which is the standard regularity assumption on the regression function m. Using the result of the Problem 3.3 in Györfi et al. (2002) dealing with binary models, we finally obtain that the sequence $a_n = n^{-\frac{2h}{2h+d}}$ is a lower minimax rate of convergence for this class of distributions and more precisely that Equation (14) holds.