Mathematical Properties of Continuous Ranked Probability Score Forecasting

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Probabilistic Forecasting

All those whose duty it is to issue regular daily forecasts know that there are times when they feel **very confident** and other times when they are **doubtful** as to coming weather. It seems to me that the condition of confidence or otherwise forms a **very important part of the prediction**.

Ernest Cook (MWR, 1906)

- Various approaches :
  - Ensemble prediction
  - Quantile regression
  - Expectile regression
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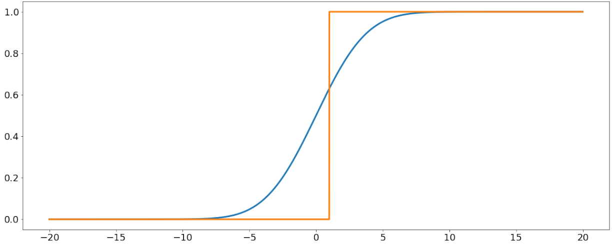
Probabilistic Forecasting Techniques

- Various approaches :
  - Ensemble prediction
  - Quantile regression
  - Expectile regression
  - **Distributional regression** : cumulative distribution function, density, quantile function, copula...
- How can we compare a distribution and an observation? $\rightarrow$ **Scoring Rules**

Continuous Ranked Probability Score

- Continuous Ranked Probability Score (CRPS) : [Matheson and Winkler, 1976]

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



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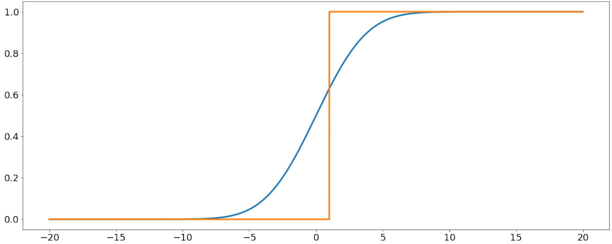

- Difference of expected scores :

$$\overline{\mathrm{CRPS}}(F, G) - \overline{\mathrm{CRPS}}(G, G) = \int_{\mathbb{R}} (F(z) - G(z))^2 \mathrm{d}z$$

$$\overline{\mathrm{CRPS}}(F, G) \geq \overline{\mathrm{CRPS}}(G, G) \text{ (strictly proper)}$$

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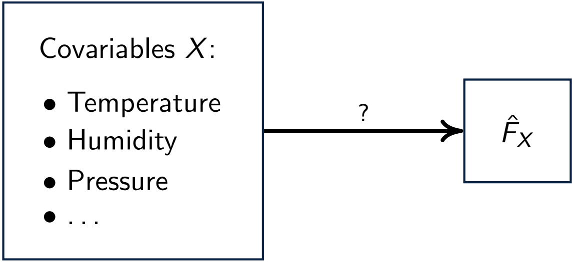
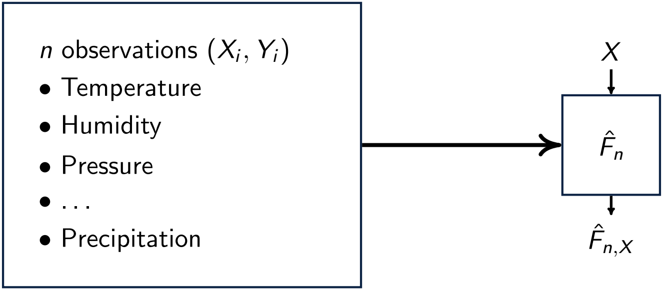
Theoretical framework

- $Y \in \mathbb{R}$ variable of interest, $X \in \mathbb{R}^d$ covariables with $(X, Y) \sim P$.
- Goal : estimate the conditional distribution of Y given X, noted F_X^*.



- In practice : estimate the conditional distribution of Y given X based on $\boldsymbol{n}$ **observations** $D_n = \{(X_i, Y_i), i \in [\![1; n]\!]\}$ where (X_i, Y_i) are assumed i.i.d. following P.



- Verification with the CRPS

Applications of this framework

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- Predict a parametric or nonparametric distribution : Censored-Shifted Gamma, Censored-GEV, EGPD, QRF, Bernstein polynomials...
- Predicted distribution represented as an ensemble of values : Random/Quantile Ensembles, Generators...

Convergence and rate of convergence

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Definition

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

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

and

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

where the infimum is taken over all distributional regression models $\hat{F}_n$ trained on D_n.

Consider the following classes :

Definition

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

i) $X \in [0, 1]^d$ P_X-a.s.;

ii) For all $x \in [0, 1]^d$, $\int_{\mathbb{R}} F^*_x(z)(1 - F^*_x(z))\mathrm{d}z \leq M$;

iii) $\|F^*_{x'} - F^*_x\|_{L^2} \leq C\|x' - x\|^h$ for all $x, x' \in [0, 1]^d$.

Remark : Conditions similar to point regression [Györfi et al., 2002].

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iii) $\boldsymbol{\|F_{x'}^* - F_x^*\|_{L^2} \leq C\|x' - x\|^h}$ **for all** $\boldsymbol{x, x'} \in [\mathbf{0}, \mathbf{1}]^{\boldsymbol{d}}$.

$$\overline{\mathrm{CRPS}}(\hat{F}_{n,X}, F_X^*) - \overline{\mathrm{CRPS}}(F_X^*, F_X^*) = \int_{\mathbb{R}} (\hat{F}_{n,X}(z) - F_X^*(z))^2 \mathrm{d}z = \|\hat{F}_{n,X} - F_X^*\|_{L^2}$$

Using knowledge from previous observations at $X = x_i$ to extrapolate the value at $X = x$ $\rightarrow$ Need regularity of F^*.

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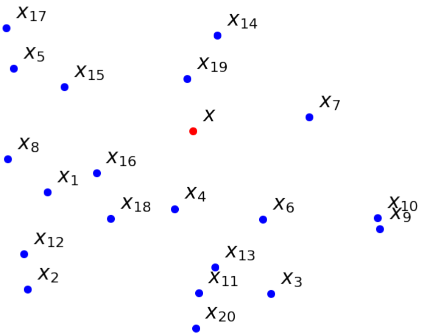
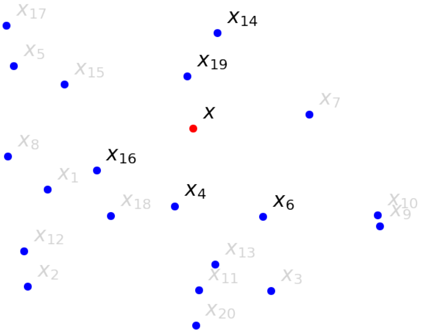


$$\hat{F}_{n,x}(z) = \frac{1}{k_n} \sum_{i=1}^{k_n} \mathbb{1}_{y_{i:n}(x) \leq z}, \quad {}_{i:n}(x) \text{ index of the } i\text{-th nearest neighbor of } x.$$

k-Nearest Neighbors



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k-Nearest Neighbors

- (L) Use a subclass with a binary response to obtain a **lower minimax rate of convergence** : $\boldsymbol{a_n = n^{-\frac{2h}{2h+d}}}$.

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Proposition

Assume $P \in \mathcal{D}^{(h,C,M)}$ and let $\hat{F}_n$ be the k-NN model. Then,

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

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 $\mathbb{R}^d$.

Theorem

For $d \geq 2$, the optimal minimax rate of convergence on the class $\mathcal{D}^{(h,C,M)}$ is $\boldsymbol{a_n = n^{-\frac{2h}{2h+d}}}$. Moreover, the k-NN algorithm reaches the optimal rate of convergence for

$$k_n = \left(\frac{Md}{2hC^2c_d^h}\right)^{\frac{d}{2h+d}} n^{\frac{2h}{2h+d}}.$$

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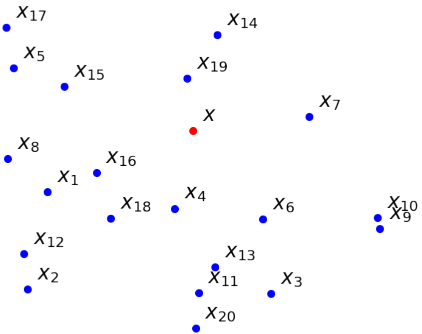
- What happens in $d = 1$?
- Interesting result but k-NN not used in practice.

Kernel Method



$$\hat{F}_{n,x}(z) = \frac{\sum_{i=1}^{n} K(\frac{x-x_i}{h_n})\mathbb{1}_{y_i \leq z}}{\sum_{i=1}^{n} K(\frac{x-x_i}{h_n})}, \text{ with } K(z) = \mathbb{1}_{\{\|z\| \leq 1\}}.$$

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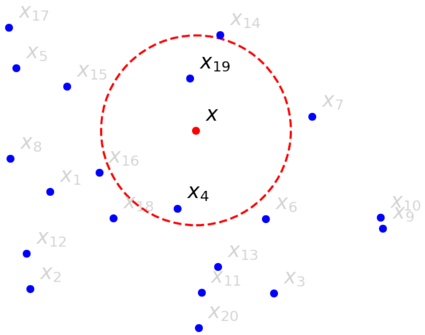

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Assume $P \in \mathcal{D}^{(h,C,M)}$ and let $\hat{F}_n$ be the naive kernel model. Then,

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

where $\tilde{c}_d$ only depends on $d \geq 1$.

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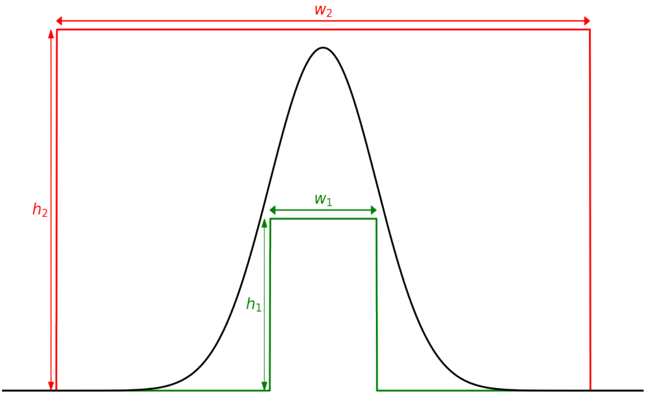
- Optimal minimax rate of convergence for any d.
- Used in practice ?

Boxed Kernel



Conclusion

- Optimal minimax rate of convergence for distributional regression.
- Upper bound on the convergence rate for k-NN and kernel methods at fixed n.
- Extension to usual weighted CRPSs.
- Perspectives :
    - Study other algorithms : Random Forests (e.g. QRF).
    - Study other definitions of convergence : other distances.
    - Adapt other classical results to the distributional regression framework.

Preprint : Mathematical Properties of Continuous Ranked Probability Score Forecasting, Pic et al. (https://arxiv.org/abs/2205.04360)

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Simulations

- $X_1, X_2 \sim \mathcal{U}([0,1])$
- $Y = X_1 + X_2 + \sigma\epsilon$ with $\epsilon \sim \mathcal{N}(0,1)$
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  $\rightarrow M = \frac{\sigma}{\sqrt{\pi}}$ ✓

  iii) $\boldsymbol{\|F_{x'}^* - F_x^*\|_{L^2} \leq C\|x' - x\|^h}$ **for all** $\boldsymbol{x, x' \in [0,1]^d}$.
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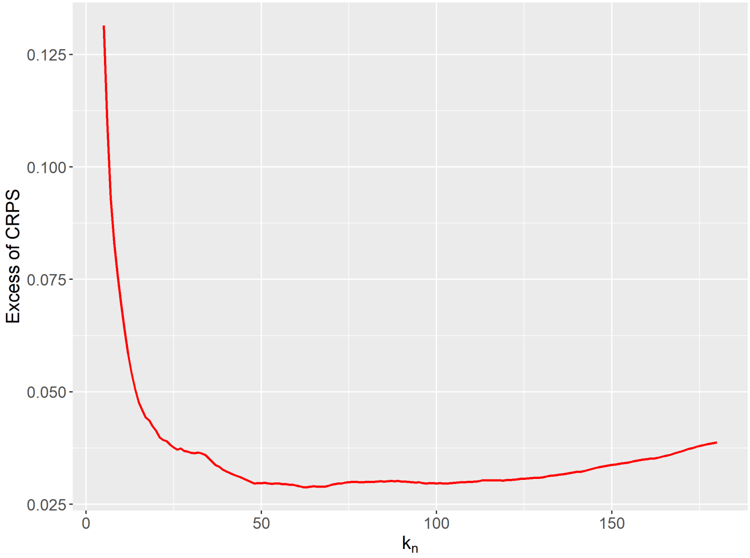
CRPS vs. k_n

Parameters : $\sigma = 1$ and $n = 200$.



Scaling of k_n with n, $\sigma = 2$

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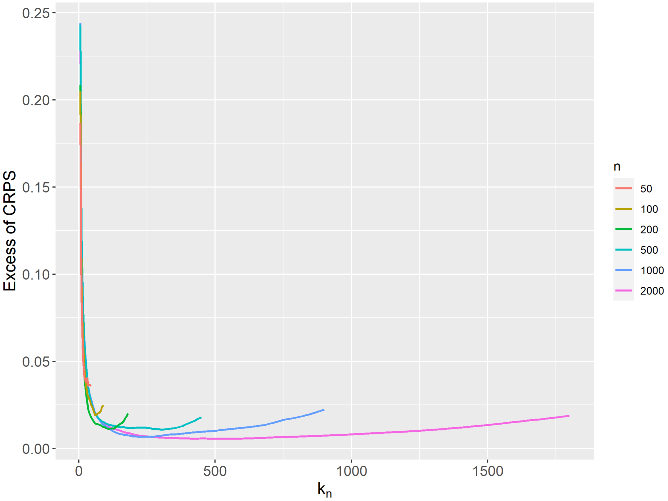

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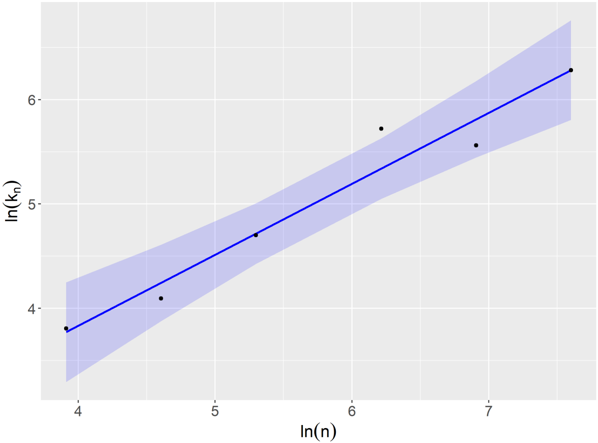

Figure: Equation : $y = 1.1 + 0.68x, \; R^2 = 0.952$

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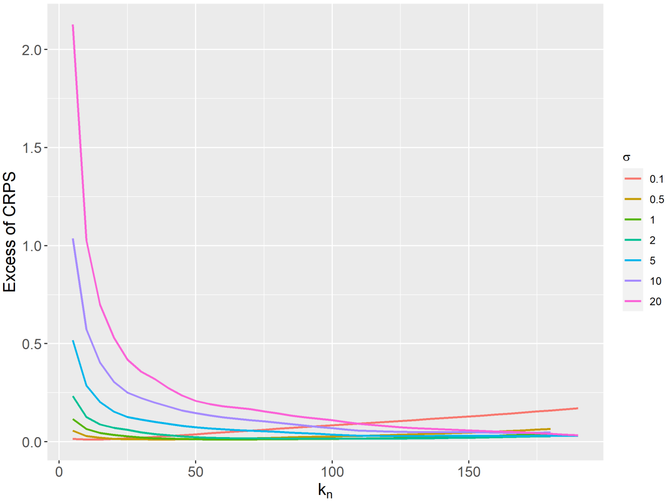

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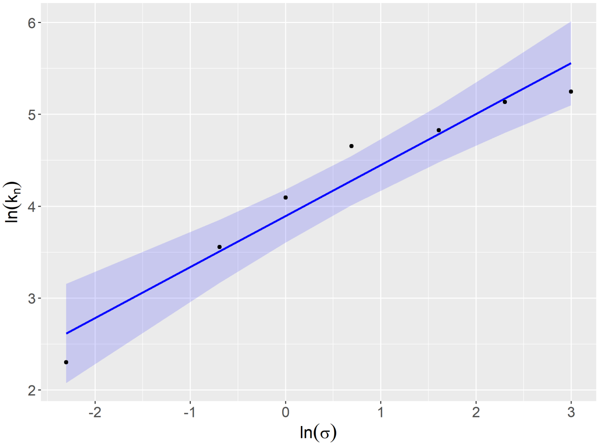

Figure: Equation : $y = 3.9 + 0.56x$, $R^2 = 0.942$