

Conformal prediction

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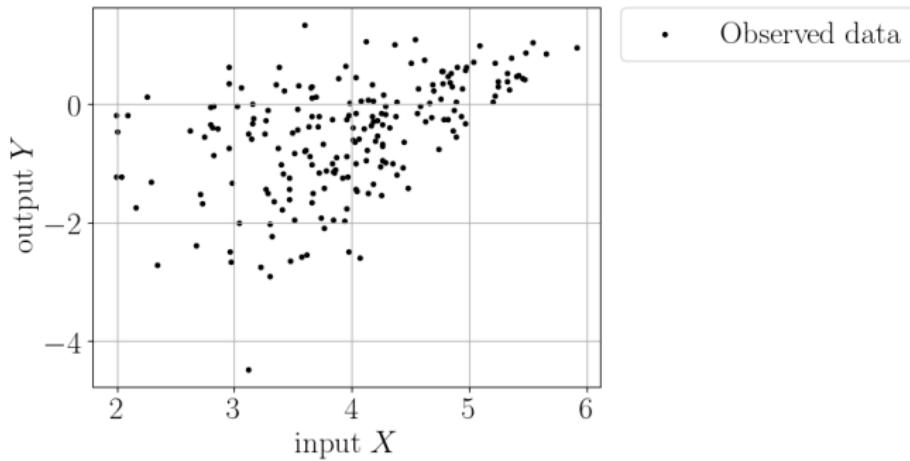
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Illustration

Data set

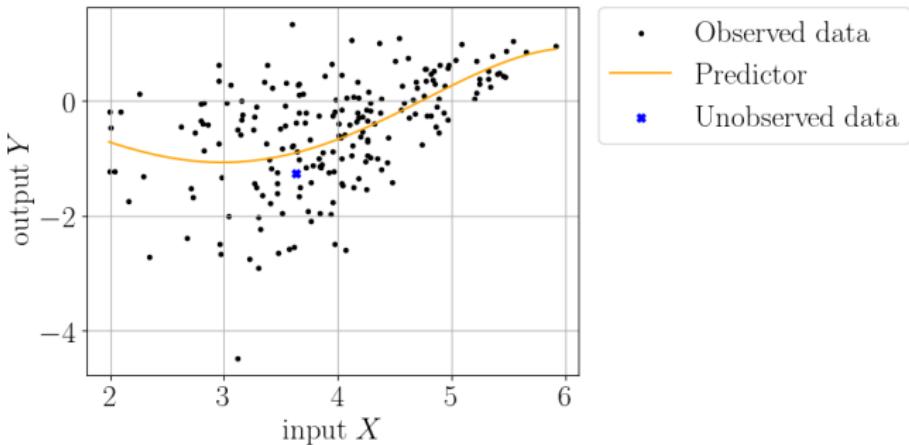
$(X_1, Y_1), \dots, (X_n, Y_n)$, independent and identically distributed as (X, Y) random variables, where $X \sim \beta(6, 3)$ and $Y|X \sim \cos(X) + (1 - \cos(X))\mathcal{N}(0, 0.5)$.



Illustration

Prediction

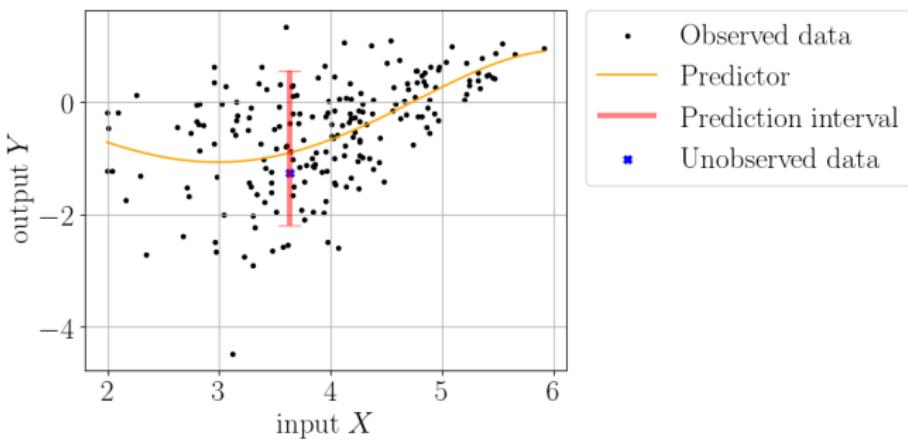
Given (X_{n+1}, Y_{n+1}) independent and identically distributed as $(X_1, Y_1), \dots, (X_n, Y_n)$, a prediction \hat{Y}_{n+1} approximates Y_{n+1} .



Illustration

Prediction region

Given (X_{n+1}, Y_{n+1}) , independent and identically distributed as $(X_1, Y_1), \dots, (X_n, Y_n)$, for a confidence control level α , a prediction region $\hat{C}_\alpha(X_{n+1})$ contains Y_{n+1} with probability greater than $1 - \alpha$.



Setup

- ▶ Data set: $(X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$, $\mathcal{X} \times \mathcal{Y}$ -valued independent and identically distributed random variables where $\mathcal{X} \subseteq \mathbb{R}$, and $\mathcal{Y} \subseteq \mathbb{R}$.
- ▶ Regression: Predict $\hat{Y}_{n+1} \approx Y_{n+1}$ provided X_{n+1} and the observed data points $(X_1, Y_1), \dots, (X_n, Y_n)$.

Confidence prediction region

For a confidence control level α , a confidence prediction region $C_\alpha(X_{n+1})$ fulfills the following

$$\mathbb{P}[Y_{n+1} \in C_\alpha(X_{n+1})] \geq 1 - \alpha.$$

Solution

Conformal prediction (Vovk, Gammerman, and Shafer, 2005).

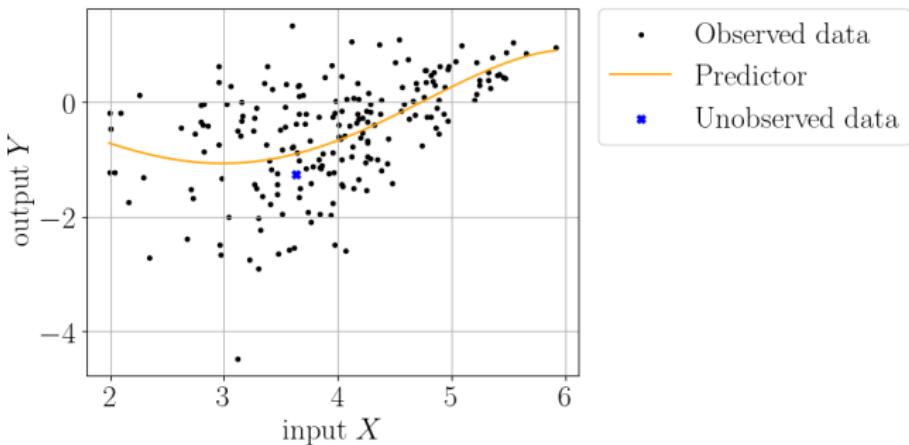
Predictor

- ▶ Feature map: $\phi(\cdot) : \mathcal{X} \mapsto \mathbb{R}^d$. For example, for every $x \in \mathbb{R}$,
 $\phi(x) = (1, x, x^2, x^3, x^4)^T$.

Ridge regression

For a data set D and a regularization parameter $\lambda \in (0, +\infty)$

$$\hat{\beta}_{\lambda;D} := \arg \min_{\beta \in \mathbb{R}^d} \frac{1}{|D|} \sum_{(x,y) \in D} (y - \phi(x)^T \beta)^2 + \lambda \|\beta\|_2^2.$$



Full conformal prediction

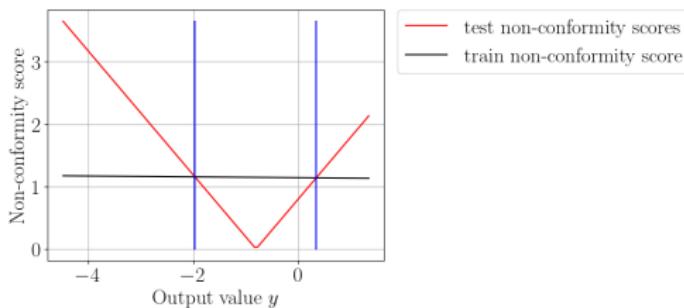
Non-conformity scores

For every $i \in \{1, \dots, n+1\}$ and every $\mathbf{y} \in \mathcal{Y}$

$$S_{D^y}(X_i, Y_i) = \left| Y_i - \phi(X_i)^T \hat{\beta}_{\lambda; D^y} \right|, \quad \text{if } 1 \leq i \leq n,$$

$$S_{D^y}(X_i, \mathbf{y}) = \left| \mathbf{y} - \phi(X_i)^T \hat{\beta}_{\lambda; D^y} \right|, \quad \text{if } i = n+1,$$

where the data set D^y is defined as $D^y := \{(X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, \mathbf{y})\}$.



- ▶ It measures the “strangeness” each data points in D^y .
- ▶ For example, $S_{D^y}(X_{n+1}, \mathbf{y})$ is the least strange for a value y around -0.7 and gets more strange for values away from -0.7 .

Full conformal prediction

Non-conformity scores

For every $i \in \{1, \dots, n+1\}$ and every $\textcolor{blue}{y} \in \mathcal{Y}$

$$S_{D^{\textcolor{blue}{y}}} (X_i, Y_i) = s \left(Y_i, \hat{f}_{D^{\textcolor{blue}{y}}} (X_i) \right), \quad \text{if } 1 \leq i \leq n,$$

$$S_{D^{\textcolor{blue}{y}}} (X_i, \textcolor{blue}{y}) = s \left(\textcolor{blue}{y}, \hat{f}_{D^{\textcolor{blue}{y}}} (X_i) \right), \quad \text{if } i = n+1,$$

where the data set $D^{\textcolor{blue}{y}}$ is defined as $D^{\textcolor{blue}{y}} := \{(X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, \textcolor{blue}{y})\}$, and $s(\cdot, \cdot) : \mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}$ is a non-conformity function.

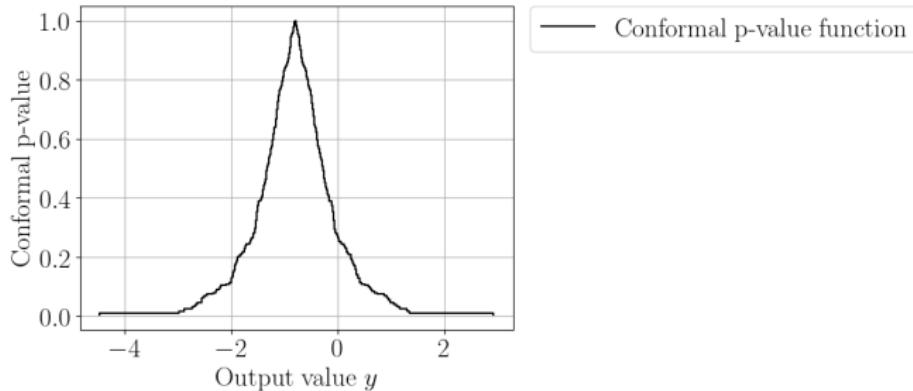
- ▶ It measures the “strangeness” each data points in $D^{\textcolor{blue}{y}}$.

Full conformal prediction

Full conformal p-value function

For every output value $y \in \mathcal{Y}$

$$\hat{\pi}_D^{\text{Full}}(X_{n+1}, y) := \frac{1 + \sum_{i=1}^n \mathbb{1}\{S_{D^y}(X_i, Y_i) \geq S_{D^y}(X_{n+1}, y)\}}{n+1}.$$



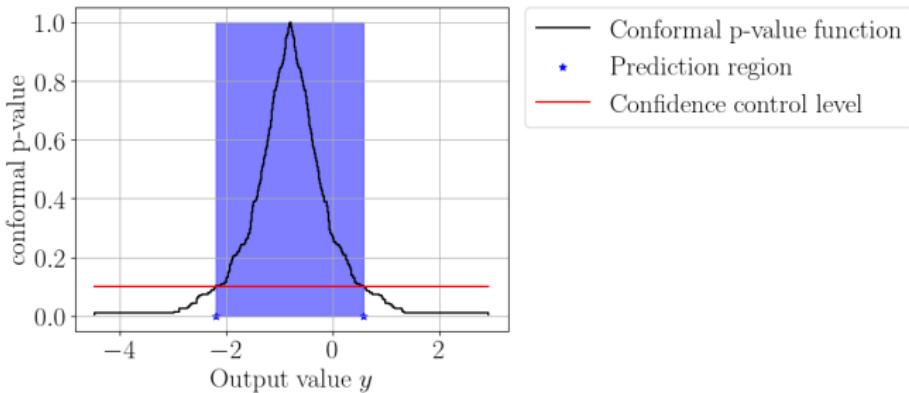
- ▶ It measures how strange is (X_{n+1}, y) relative the other data points in D^y .
- ▶ For example, it is relatively the least strange for a value y around -0.7 , and relatively more strange for values y far from -0.7 .

Full conformal prediction

Full conformal prediction region (FCPR)

For a **confidence control level** α , the FCPR $\hat{C}_\alpha^{\text{Full}}(X_{n+1})$ is defined as

$$\hat{C}_\alpha^{\text{Full}}(X_{n+1}) := \left\{ y \in \mathcal{Y} : \hat{\pi}_D^{\text{Full}}(X_{n+1}, y) > \alpha \right\}.$$



- It is the set of the values of y , such (X_{n+1}, y) is relatively not too strange.

Explicit computation

Linear predictor

If the predictor \hat{f}_{D^y} is linear then for every $x \in \mathcal{X}$, there exists a vector $\hat{A}(\mathbf{X}, x) \in \mathbb{R}^{n+1}$ such that

$$\hat{f}_{D^y}(x) = \hat{A}(\mathbf{X}, x)^T \mathbf{Y}^y,$$

where $\mathbf{X} = (X_1, \dots, X_n, X_{n+1})^T \in \mathbb{R}^{n+1}$ and $\mathbf{Y}^y = (Y_1, \dots, Y_n, y)^T \in \mathbb{R}^{n+1}$.

Conformal p-value function

Moreover, there exist vectors $a, b \in \mathbb{R}^{n+1}$ dependent on $(X_1, Y_1), \dots, (X_n, Y_n)$ and X_{n+1} , such that for every $y \in \mathcal{Y}$,

$$\begin{aligned}\widehat{\pi}_D^{\text{Full}}(X_{n+1}, y) &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\{S_{D^y}(X_i, Y_i) \geq S_{D^y}(X_{n+1}, y)\}}{n+1} \\ &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\left\{\left|Y_i - \hat{f}_{D^y}(X_i)\right| \geq \left|y - \hat{f}_{D^y}(X_{n+1})\right|\right\}}{n+1} \\ &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\{|a_i + b_i y| \geq |a_{n+1} + b_{n+1} y|\}}{n+1}.\end{aligned}$$

Explicit computation

Linear predictor

For example, for every $x \in \mathcal{X}$,

$$\hat{f}_{D^y}(x) = \phi(x)^T \left(\frac{1}{n+1} \phi(\mathbf{X})^T \phi(\mathbf{X}) + 2\lambda I_p \right)^{-1} \left(\frac{1}{n+1} \phi(\mathbf{X})^T \right) \mathbf{Y}^y,$$

where $\phi(\mathbf{X}) = [\phi(X_1), \dots, \phi(X_n), \phi(X_{n+1})]^T \in \mathbb{R}^{n+1 \times p}$.

Conformal p-value function

Moreover, there exist vectors $a, b \in \mathbb{R}^{n+1}$ dependent on $(X_1, Y_1), \dots, (X_n, Y_n)$ and X_{n+1} , such that for every $y \in \mathcal{Y}$,

$$\begin{aligned}\hat{\pi}_D^{\text{Full}}(X_{n+1}, y) &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\{S_{D^y}(X_i, Y_i) \geq S_{D^y}(X_{n+1}, y)\}}{n+1} \\ &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\left\{\left|Y_i - \hat{f}_{D^y}(X_i)\right| \geq \left|y - \hat{f}_{D^y}(X_{n+1})\right|\right\}}{n+1} \\ &:= \frac{1 + \sum_{i=1}^n \mathbb{1}\{|a_i + b_i y| \geq |a_{n+1} + b_{n+1} y|\}}{n+1}.\end{aligned}$$

Full conformal prediction

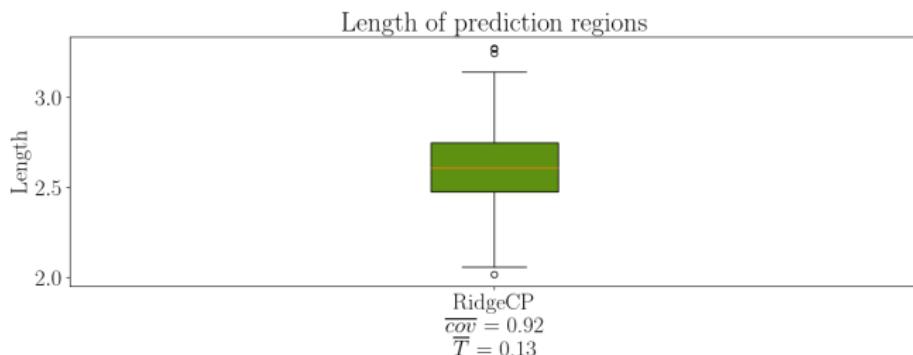
Coverage guarantee

If $(X_1, Y_1), \dots, (X_{n+1}, Y_{n+1})$ are exchangeable, then the FCPR $\hat{C}_\alpha^{\text{Full}}(X_{n+1})$ enjoys the following guarantee,

$$\mathbb{P} \left[Y_{n+1} \in \hat{C}_\alpha^{\text{Full}}(X_{n+1}) \right] \geq 1 - \alpha.$$

Moreover $S_{D^{Y_{n+1}}}(X_1, Y_1), \dots, S_{D^{Y_{n+1}}}(X_{n+1}, Y_{n+1})$ are almost surely distinct, then

$$\mathbb{P} \left[Y_{n+1} \in \hat{C}_\alpha^{\text{Full}}(X_{n+1}) \right] \leq 1 - \alpha + \frac{1}{n+1}.$$



- \bar{cov} which is an empirical estimation of the coverage probability is indeed not far from $0.9 = 1 - \alpha$.

Proof (Part 1)

Since $\hat{f}_{D^{Y_{n+1}}}^*$ is invariant to permutation of the data points in $D^{Y_{n+1}}$, and $(X_1, Y_1), \dots, (X_{n+1}, Y_{n+1})$ are exchangeable, it follows that $S_{D^{Y_{n+1}}}(X_1, Y_1), \dots, S_{D^{Y_{n+1}}}(X_{n+1}, Y_{n+1})$ are exchangeable.

Let us note for every $i \in \{1, \dots, n+1\}$, $S_i := S_{D^{Y_{n+1}}}(X_i, Y_i)$, and sort them $S_{(1)} \geq \dots \geq S_{(n+1)}$. Let us consider the following set

$$\begin{aligned}\text{Strange}(\alpha) &:= \left\{ i \in \{1, \dots, n+1\}, \sum_{j=1}^{n+1} \mathbb{1}\{S_j \geq S_i\} \leq \alpha(n+1) \right\} \\ &= \left\{ i \in \{1, \dots, n+1\}, \sum_{j=1}^{n+1} \mathbb{1}\{S_{(j)} \geq S_{(i)}\} \leq \alpha(n+1) \right\} \\ &\subseteq \{i \in \{1, \dots, n+1\}, (i) \leq \alpha(n+1)\} \\ &\subseteq \{i \in \{1, \dots, n+1\}, (i) \leq \lfloor \alpha(n+1) \rfloor\}.\end{aligned}$$

It follows that

$$\text{Card}(\text{Strange}(\alpha)) \leq \sum_{i=1}^{n+1} \mathbb{1}\{(i) \leq \lfloor \alpha(n+1) \rfloor\} \leq \lfloor \alpha(n+1) \rfloor.$$

Proof (Part 2)

Let us consider the probability of not covering

$$\begin{aligned} & \mathbb{P} \left[Y_{n+1} \notin \hat{C}_\alpha^{\text{Full}}(X_{n+1}) \right] \\ &= \mathbb{P} [\hat{\pi}_D(X_{n+1}, Y_{n+1}) \leq \alpha] \\ &= \mathbb{P} \left[\frac{\sum_{i=1}^{n+1} \mathbb{1} \left\{ S_{D Y_{n+1}}(X_i, Y_i) \geq S_{D Y_{n+1}}(X_{n+1}, Y_{n+1}) \right\}}{n+1} \leq \alpha \right] \\ &= \mathbb{P} [n+1 \in \text{Strange}(\alpha)], \end{aligned}$$

and since S_1, \dots, S_{n+1} are exchangeable

$$\begin{aligned} \mathbb{P} [n+1 \in \text{Strange}(\alpha)] &= \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{P} [i \in \text{Strange}(\alpha)] \\ &= \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{E} [\mathbb{1} \{i \in \text{Strange}(\alpha)\}] \\ &= \frac{1}{n+1} \mathbb{E} \left[\sum_{i=1}^{n+1} \mathbb{1} \{i \in \text{Strange}(\alpha)\} \right] \\ &= \frac{\mathbb{E} [\text{Card}(\text{Strange}(\alpha))]}{n+1} \leq \frac{\lfloor \alpha(n+1) \rfloor}{n+1} \leq \alpha. \end{aligned}$$

Proof (Part 3)

Let us consider the case where S_1, \dots, S_{n+1} are almost surely distinct. It follows that almost surely $S_{(1)} > \dots > S_{(n+1)}$. Going back to set of strange points

$$\begin{aligned}\text{Strange}(\alpha) &:= \left\{ i \in \{1, \dots, n+1\}, \sum_{j=1}^{n+1} \mathbb{1} \{S_j \geq S_i\} \leq \alpha(n+1) \right\} \\ &= \left\{ i \in \{1, \dots, n+1\}, \sum_{j=1}^{n+1} \mathbb{1} \{S_{(j)} \geq S_{(i)}\} \leq \alpha(n+1) \right\} \\ &= \{i \in \{1, \dots, n+1\}, (i) \leq \alpha(n+1)\} \\ &\supseteq \{i \in \{1, \dots, n+1\}, (i) \leq \lceil \alpha(n+1) \rceil\}.\end{aligned}$$

It follows that

$$\text{Card}(\text{Strange}(\alpha)) \geq \sum_{i=1}^{n+1} \mathbb{1} \{(i) \leq \lceil \alpha(n+1) \rceil\} = \lceil \alpha(n+1) \rceil.$$

Therefore, following a similar argument as before

$$\mathbb{P} \left[Y_{n+1} \notin \hat{C}_\alpha^{\text{Full}}(X_{n+1}) \right] \geq \frac{\lceil \alpha(n+1) \rceil}{n+1} \geq \frac{\alpha(n+1)-1}{n+1} \geq \alpha - \frac{1}{n+1}.$$

Practical considerations

Full conformal prediction region depends on

- ▶ the confidence control level $1 - \alpha$, and
- ▶ the quality of the predictor $\hat{f}_\lambda : \mathcal{X} \mapsto \mathcal{Y}$.

In general, computing the full conformal prediction exactly is too computationally costly.

- ▶ In fact, a brute force approach requires training as many predictors as the cardinality of the space of output values \mathcal{Y} , which in regression is $+\infty$.

Commonly-used computationally affordable approximation are

- ▶ Split conformal prediction (Papadopoulos, 2008),
- ▶ Cross conformal prediction (Barber et al., 2021), and
- ▶ Stable conformal prediction (Ndiaye, 2022).

We devised a new approximation with better guarantees (Razafindrakoto, Celisse, and Lacaille, 2026) for kernel regression with regularization.

Non-conformity scores (split conformal)

Data sets

For $n_{\text{train}}, n_{\text{cal}} \in \mathbb{N}$ such that $n_{\text{train}} + n_{\text{cal}} = n$,

- ▶ the calibration data set D_{cal} is defined as $D_{\text{cal}} := \{(X_1, Y_1), \dots, (X_{n_{\text{cal}}}, Y_{n_{\text{cal}}})\}$,
- ▶ the training data set D_{train} is defined as
$$D_{\text{train}} := \{(X_{n_{\text{cal}}+1}, Y_{n_{\text{cal}}+1}), \dots, (X_n, Y_n)\}.$$

Non-conformity scores

For every $i \in \{1, \dots, n_{\text{cal}}\}$ and every $y \in \mathcal{Y}$

$$\begin{aligned} S_{D_{\text{train}}} (X_i, Y_i) &= \left| Y_i - X_i^T \hat{\beta}_{\lambda; D_{\text{train}}} \right|, & \text{if } 1 \leq i \leq n_{\text{cal}}, \\ S_{D_{\text{train}}} (X_i, y) &= \left| y - X_i^T \hat{\beta}_{\lambda; D_{\text{train}}} \right|, & \text{if } i = n + 1. \end{aligned}$$

- ▶ Pros: Only need to train one predictor.
- ▶ Cons: Less points for training and less non-conformity scores.

Split conformal prediction

Split conformal p-value function

For every output value $y \in \mathcal{Y}$

$$\hat{\pi}_D^{\text{Split}}(X_{n+1}, y) := \frac{1 + \sum_{i=1}^{n_{\text{cal}}} \mathbb{1}\{S_{D_{\text{train}}}(X_i, Y_i) \geq S_{D_{\text{train}}}(X_{n+1}, y)\}}{n_{\text{cal}} + 1}.$$

Split conformal prediction region (SCPR)

For a confidence control level α , the SCPR $\hat{C}_{\alpha}^{\text{Split}}(X_{n+1})$ is defined as

$$\begin{aligned}\hat{C}_{\alpha}^{\text{Split}}(X_{n+1}) &:= \left\{ y \in \mathcal{Y}, \hat{\pi}_D^{\text{Split}}(X_{n+1}, y) > \alpha \right\} \\ &= \left[X_{n+1}^T \hat{\beta}_{\lambda; D_{\text{train}}} - \left| Y_{(i_{n,\alpha})} - X_{(i_{n,\alpha})}^T \hat{\beta}_{\lambda; D_{\text{train}}} \right|, \right. \\ &\quad \left. X_{n+1}^T \hat{\beta}_{\lambda; D_{\text{train}}} + \left| Y_{(i_{n,\alpha})} - X_{(i_{n,\alpha})}^T \hat{\beta}_{\lambda; D_{\text{train}}} \right| \right],\end{aligned}$$

where $|Y_{(1)} - X_{(1)}^T \hat{\beta}_{\lambda; D_{\text{train}}}| \leq \dots \leq |Y_{(n_{\text{cal}})} - X_{(n_{\text{cal}})}^T \hat{\beta}_{\lambda; D_{\text{train}}}|$ and
 $i_{n,\alpha} = \lceil (n_{\text{cal}} + 1)(1 - \alpha) \rceil$.

Recap

- ▶ Formulating confidence prediction regions with conformal prediction,
- ▶ Computing split conformal prediction regions.

Reference

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- [5] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer. *Algorithmic learning in a random world*. Vol. 29. Springer, 2005.