# Conformal prediction

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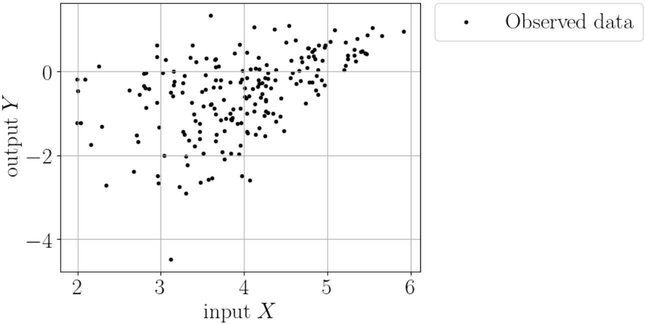
# Illustration

## Data set

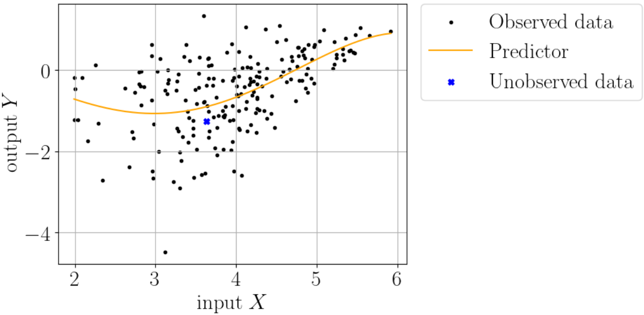
$(X_1, Y_1), \ldots, (X_n, Y_n)$, independent and identically distributed as $(X, Y)$ random variables, where $X \sim \beta(6, 3)$ and $Y|X \sim \cos(X) + (1 - \cos(X))\mathcal{N}(0, 0.5)$.



# Illustration

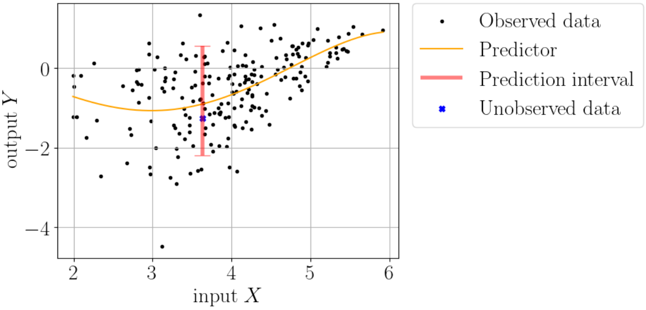
## Point prediction

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



## Prediction region

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



# Setup

- Data set: $(X_1, Y_1), \ldots, (X_n, Y_n)$, $(X_{n+1}, Y_{n+1})$, $\mathcal{X} \times \mathcal{Y}$-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 $(X_1, Y_1), \ldots, (X_n, Y_n)$.

## Confidence prediction region

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

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

## Solution

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

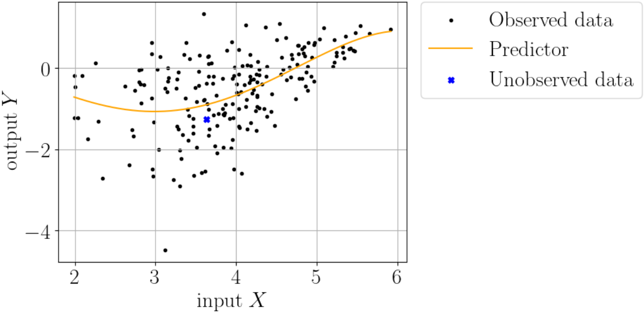
# Predictor

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

## Ridge regression

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

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



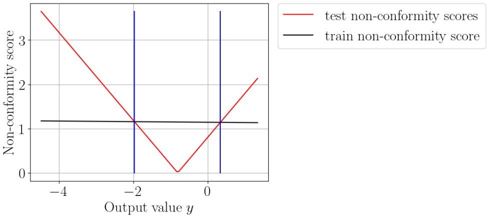
# Full conformal prediction

## Non-conformity scores

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

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

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



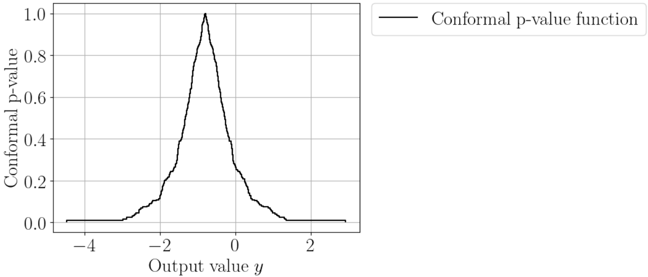

- It measures the "strangeness" each data points in $D^y$.
- For example, $S_{D^y}(X_{n+1}, y)$ is the least strange for a value $y$ around $-0.7$ and gets more strange for values away from $-0.7$.

# Full conformal prediction

## Full conformal p-value function

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

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



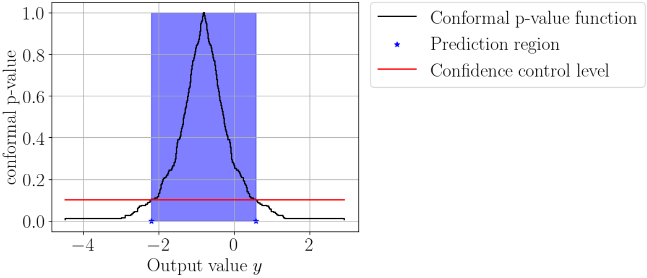

- It measures how strange is $(X_{n+1}, y)$ relative the other data points in $D^y$.
- For example, it is relatively the least strange for a value $y$ around $-0.7$, and relatively more strange for values $y$ far from $-0.7$.

# Full conformal prediction

## Full conformal prediction region (FCPR)

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

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




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

# Full conformal prediction

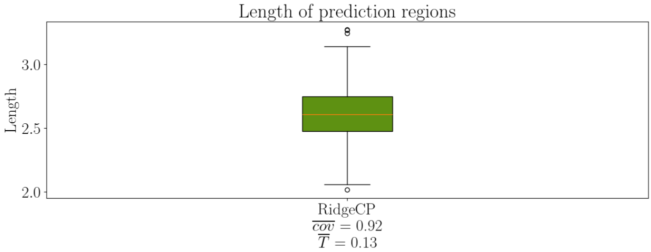
## Coverage guarantee

The FCPR $\hat{C}_{\alpha}^{\mathrm{Full}}(X_{n+1})$ enjoys the following guarantee

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

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

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




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

# Practical considerations

- In general, computing the full conformal prediction exactly is too computationaly 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 computationaly afordable approximation are Split conformal prediction (Papadopoulos, 2008), cross conformal prediction (Barber et al., 2021), and (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 $D_{\text{cal}}$ is defined as $D_{\text{cal}} := \{(X_1, Y_1), \ldots, (X_{n_{\text{cal}}}, Y_{n_{\text{cal}}})\}$,
- the training data set $D_{\text{train}}$ is defined as $D_{\text{train}} := \left\{\left(X_{n_{\text{cal}}+1}, Y_{n_{\text{cal}}+1}\right), \ldots, (X_n, Y_n)\right\}$.

## Non-conformity scores

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

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

- 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 $y \in \mathcal{Y}$

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

## Split conformal prediction region (SCPR)

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

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

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

# 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.