Conformal prediction

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M2 Tide, 9 Janvier 2026

Illustration

[TODO Here show a figure a describe the data generating distribution.]

Illustration

[TODO Here show a figure of the unobserved point.]

Illustration

[TODO Here show the predictor]

Illustration

[TODO Here show the prediction region.]

Setup

- Data:
- Predictor:

Confidence prediction region

Solution

Conformal prediction

Ridge regression

Non-conformity scores

Ridge regression

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

Non-conformity scores

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

[TODO Put a figure here]

Full conformal prediction

Full conformal p-value function

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

Full conformal prediction region

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

[TODO Put a figure here]

Non-conformity scores (split conformal)

- Data sets:

Non-conformity scores

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

Split conformal p-value function

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

Split conformal prediction

Split conformal prediction region

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

Recap

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

Reference