Conformal prediction

Statistical Learning
CLAMSES - University of Milano-Bicocca

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References

- Lei, G'Sell, Rinaldo, Tibshirani, Wasserman (2018)
  Distribution-free predictive inference for regression.
  JASA,113:1094–1111

Suppose we have fitted a Gaussian linear model based on the training data $(\mathbf{y}, \mathbf{X})$, obtaining the estimates

$$\hat{\beta} = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{y}, \quad \hat{\sigma}^2 = \|\mathbf{y} - \mathbf{X}\hat{\beta}\|^2/(n-p)$$

There are (at least) two levels at which we can make predictions

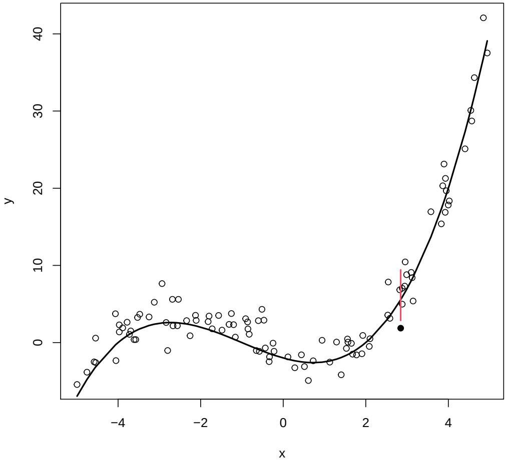
1. A *point prediction* is a single best guess about what a new Y will be when $X = x$
2. A *prediction interval*

$$C_\alpha(x) = x^t\hat{\beta} \pm t_{n-p}^{1-\alpha/2}\hat{\sigma}\sqrt{x^t(\mathbf{X}^t\mathbf{X})^{-1}x + 1}$$

for $Y|X = x$ with $(1-\alpha)$ *conditional coverage* guarantee, i.e.

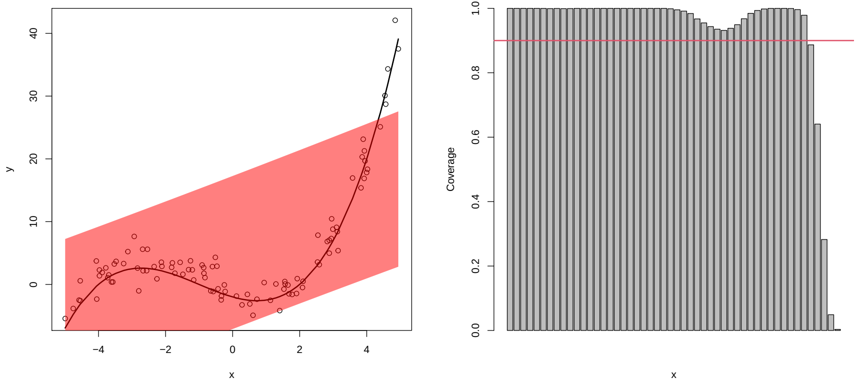
$$\mathrm{P}(Y \in C_\alpha(x)|X = x) = 1 - \alpha$$

where the probability is with respect to the training data $(X_1, Y_1), \ldots, (X_n, Y_n)$, and the new response Y at a fixed test point $X = x$



$$f(x) = \frac{1}{4}(x+4)(x+1)(x-2)$$

Model miss-specification



$$1 - \alpha = 90\%, \text{ marginal coverage} \approx 93\%$$

Marginal and conditional coverage

- $(X, Y) \in \mathbb{R}^p \times \mathbb{R}$ follows some *unknown* joint distribution P_{XY}
- Training $(X_1, Y_1), \ldots, (X_n, Y_n)$ and test (X_{n+1}, Y_{n+1}) i.i.d. (X, Y)
- C_α satisfies *distribution-free marginal coverage* at level $1 - \alpha$ if

$$\mathrm{P}(Y_{n+1} \in C_\alpha(X_{n+1})) \geq 1 - \alpha \qquad \forall\ P_{XY}$$

  where the probability is w.r.t. $(X_1, Y_1), \ldots, (X_n, Y_n)$ and (X_{n+1}, Y_{n+1})
- C_α satisfies *distribution-free conditional coverage* at level $1 - \alpha$ if

$$\mathrm{P}(Y_{n+1} \in C_\alpha(X_{n+1}) | X_{n+1} = x) \geq 1 - \alpha \qquad \forall\ P_{XY},\ \ \forall\ x$$

  where the probability is w.r.t. $(X_1, Y_1), \ldots, (X_n, Y_n)$, and Y_{n+1} at a fixed test point $X_{n+1} = x$

Conformal prediction

Conformal prediction (Vovk, Gammerman, Saunders, Vapnik, 1996-1999) is a general framework for constructing prediction intervals by using *any* algorithm with finite sample and distribution-free *exact* marginal coverage, i.e.

$$\mathrm{P}(Y_{n+1} \in C_\alpha(X_{n+1})) = 1 - \alpha \qquad \forall\ P_{XY}$$

Two main versions:

- *Full* conformal prediction
- *Split* conformal prediction

Algorithm 1 Full conformal prediction

Require: Training $(x_1, y_1), \ldots, (x_n, y_n)$, test x_{n+1}, algorithm $\hat{\mu}$, level α, grid of values $\mathcal{Y} = \{y, y', y'', \ldots\}$

for $y \in \mathcal{Y}$ **do**

  Train $\hat{\mu}^y(x) = \hat{\mu}(x; (x_1, y_1), \ldots, (x_n, y_n), (x_{n+1}, y))$

  Compute $R_i^y = |y_i - \hat{\mu}^y(x_i)|$ for $i = 1, \ldots, n$

  Sort $R_1^y, \ldots, R_n^y$ in increasing order: $R_{(1)}^y \leq \ldots \leq R_{(n)}^y$

  Compute $R_\alpha^y = R_{(k)}^y$ with $k = \lceil (1-\alpha)(n+1) \rceil$

  Compute $R^y = |y - \hat{\mu}^y(x_{n+1})|$

end for

$C_\alpha(x_{n+1}) = \{y \in \mathcal{Y} : R^y \leq R_\alpha^y\}$

- Assume that (X_i, Y_i), $i = 1, \ldots, n+1$ are i.i.d. from a probability distribution P_{XY} on the sample space $\mathbb{R}^p \times \mathbb{R}$. This is the only assumption of the method
- The prediction interval

  $$C_\alpha(x_{n+1}) = \{y \in \mathbb{R} : R^y \leq R^y_\alpha\},$$

  satisfies

  $$\mathrm{P}(Y_{n+1} \in C_\alpha(X_{n+1})) = 1 - \alpha$$

  if and only if $\alpha \in \{1/(n+1), 2/(n+1), \ldots, n/(n+1)\}$
- Informally, the null hypothesis that the random variable Y_{n+1} will have the outcome y, i.e.

  $$H_y : Y_{n+1} = y$$

  is rejected when $R^y > R^y_\alpha$

Algorithm 2 Split conformal prediction

Require: Training $(x_1, y_1), \ldots, (x_n, y_n)$, x_{n+1}, algorithm $\hat{\mu}$, validation sample size m, level α

1: Split $\{1, \ldots, n\}$ into L of size w and I of size $m = n - w$
2: Train $\hat{\mu}_L(x) = \hat{\mu}(x; (x_l, y_l), l \in L)$
3: Compute $R_i = |y_i - \hat{\mu}_L(x_i)|$ for $i \in I$
4: Sort $\{R_i, i \in I\}$ in increasing order: $R_{(1)} \leq \ldots \leq R_{(m)}$
5: Compute $R_\alpha = R_{(k)}$ with $k = \lceil (1 - \alpha)(m + 1) \rceil$

$$\begin{aligned} C_\alpha(x_{n+1}) &= \{y \in \mathbb{R} : |y - \hat{\mu}_L(x_{n+1})| \leq R_\alpha\} \\ &= [\hat{\mu}_L(x_{n+1}) - R_\alpha, \hat{\mu}_L(x_{n+1}) + R_\alpha] \end{aligned}$$

- Assume that (X_i, Y_i), $i = 1, \ldots, n+1$ are i.i.d. from a probability distribution P_{XY} on the sample space $\mathbb{R}^p \times \mathbb{R}$
- The prediction interval

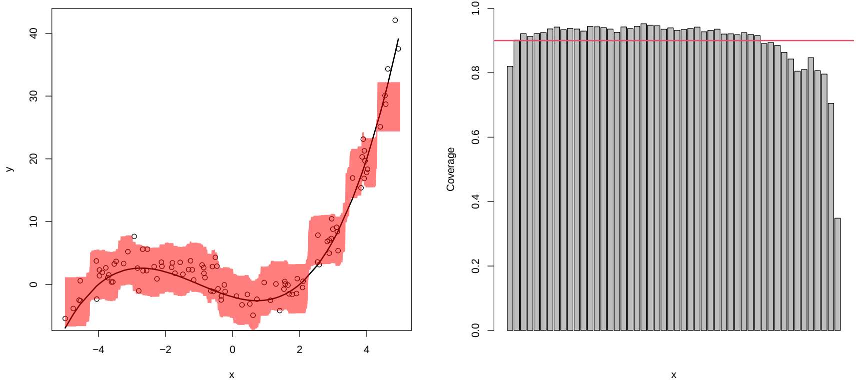
$$C_\alpha(x_{n+1}) = [\hat{\mu}_L(x_{n+1}) - R_\alpha, \hat{\mu}_L(x_{n+1}) + R_\alpha]$$

  satisfies

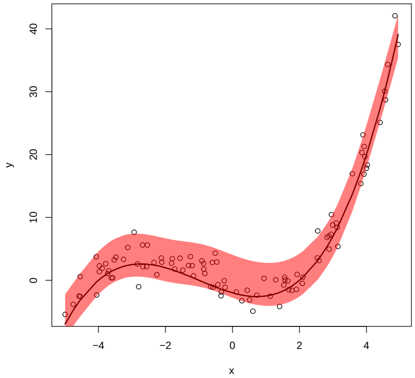
$$\mathrm{P}(Y_{n+1} \in C_\alpha(X_{n+1})) = 1 - \alpha$$

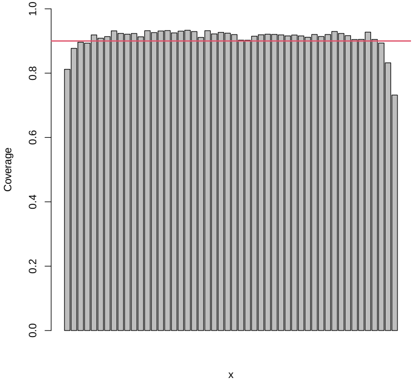
  if and only if $\alpha \in \{1/(m+1), 2/(m+1), \ldots, m/(m+1)\}$
- Note that in computing the critical value $R_\alpha = R_{(k)}$ with $k = \lceil (1-\alpha)(m+1) \rceil$, we need to have $k \leq m$, which happens if $\alpha \geq 1/(m+1)$ (otherwise if $k > m$ we need to set $R_\alpha = +\infty$)

Random Forest



Smoothing splines





Conformity scores

- In the previous algorithm we used a statistic, called *conformity score*, which is the absolute value of the residual

$$R_i = |y_i - \hat{\mu}_L(x_i)|, \quad i \in I$$

where $\hat{\mu}_L$ is an estimator of $\mathbb{E}(Y \mid X)$ based on $\{(X_i, Y_i), i \in L\}$

- The oracle knows the conditional distribution of $Y \mid X$. The oracle prediction interval

$$C^*_\alpha(x) = [q^{\alpha/2}(x), q^{1-\alpha/2}(x)]$$

where $q^\gamma(x)$ is the γ-quantile of $Y \mid X = x$, guarantees exact conditional coverage

$$\mathrm{P}(Y \in C^*_\alpha(X)|X = x) = 1 - \alpha \quad \forall\ x$$

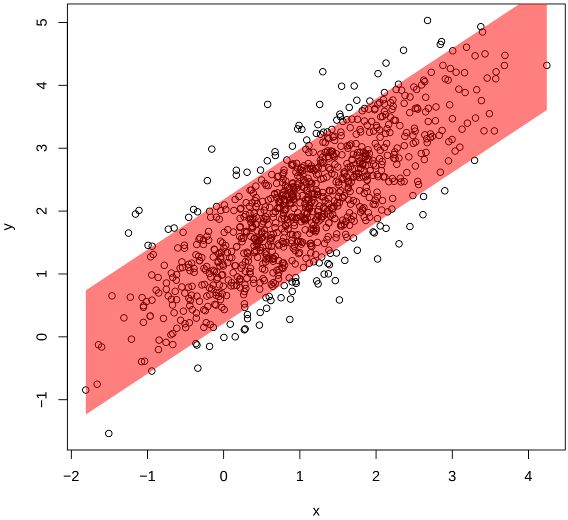
Suppose that

$$\begin{pmatrix} Y \\ X \end{pmatrix} \sim N\left(\begin{pmatrix} \mu_y \\ \mu_x \end{pmatrix}, \begin{pmatrix} \sigma_y^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_x^2 \end{pmatrix}\right)$$

then the conditional distribution of $Y \mid X = x$ is

$$(Y|X = x) \sim N\left(\mu_y + \rho\frac{\sigma_y}{\sigma_x}(x - \mu_x), \sigma_y^2(1 - \rho^2)\right)$$

from which we can compute the quantile $q^\gamma(x)$



$C^*_\alpha(x) = [q^{\alpha/2}(x), q^{1-\alpha/2}(x)]$ as a function of x

Conformal quantile regression

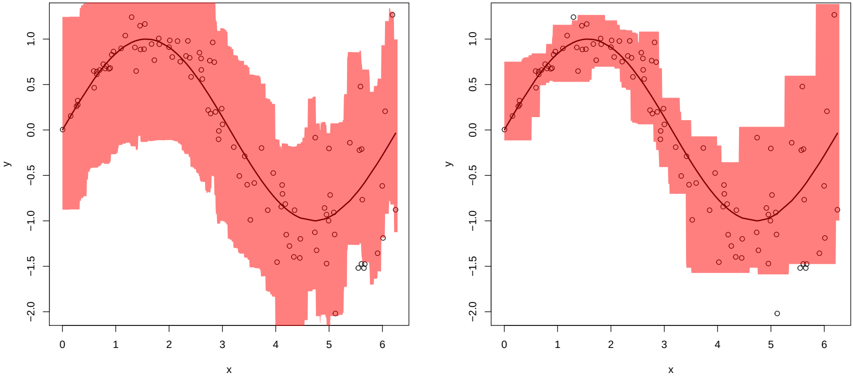
- Compute conformity scores

$$R_i = \max\left\{\hat{q}_L^{\gamma}(X_i) - Y_i, Y_i - \hat{q}_L^{1-\gamma}(X_i)\right\}, \quad i \in I$$

  where $\hat{q}_L^{\gamma}$ is an estimator of the γ-quantile of $Y \mid X$ based on $\{(X_i, Y_i), i \in L\}$
- Sort $\{R_i, i \in I\}$ in increasing order, obtaining $R_{(1)} \leq \ldots \leq R_{(m)}$, and compute $R_\alpha = R_{(k)}$ with $k = \lceil (1-\alpha)(m+1) \rceil$
- Compute the prediction interval

$$\begin{aligned} C_\alpha(x_{n+1}) &= \{y \in \mathbb{R} : \max\left\{\hat{q}_L^{\gamma}(x_{n+1}) - y, y - \hat{q}_L^{1-\gamma}(x_{n+i})\right\} \leq R_\alpha\} \\ &= [\hat{q}_L^{\gamma}(x_{n+1}) - R_\alpha, \hat{q}_L^{1-\gamma}(x_{n+1}) + R_\alpha] \end{aligned}$$

  or $C_\alpha(x_{n+1}) = \emptyset$ if $R_\alpha < (1/2)(\hat{q}_L^{\gamma}(x_{n+1}) - \hat{q}_L^{1-\gamma}(x_{n+1}))$



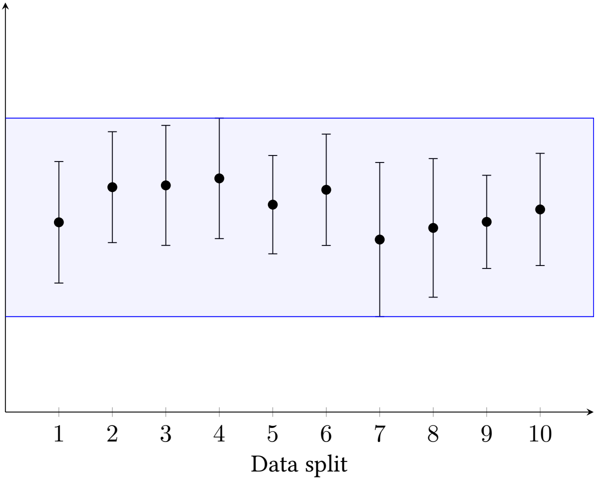
$$X_i \sim U(0, 2\pi), \epsilon_i \sim N(0,1), Y_i = \sin(X_i) + \frac{\pi|X_i|}{20}\epsilon_i$$

Multi-split conformal prediction

Algorithm

1. Choose a number B of splits
2. Choose a threshold $\tau \in \{0, 1/B, 2/B, \ldots, (B-1)/B\}$
3. Compute B split conformal prediction intervals with coverage level $1-\beta$
$$C_\beta^{[1]}(x_{n+1}), \ldots, C_\beta^{[B]}(x_{n+1})$$
where
$$\beta = \alpha(1-\tau)$$
4. Compute the aggregated prediction interval
$$C_\alpha^\tau(x_{n+1}) = \{y \in \mathbb{R} : \Pi_\beta^y > \tau\}$$
with
$$\Pi_\beta^y = \frac{1}{B} \sum_{b=1}^{B} \mathbb{1}\{y \in C_\beta^{[b]}(x_{n+1})\}$$

$\tau = 0 \quad \beta = 10\%$



- The multi-split prediction interval guarantees

$$\mathrm{P}(Y_{n+1} \in C_\alpha^\tau(X_{n+1})) \geq 1 - \alpha \qquad \forall\ P_{XY}$$

- The parameter τ can be regarded as a tuning parameter, and proper choice of τ is essential for good performance
- On the one hand, setting $\tau = 1 - 1/B$ gives the Bonferroni-intersection method with $C_\alpha^{(B-1)/B} = \bigcap_b C_{\alpha/B}^{[b]}$.
- On the other hand, setting $\tau = 0$ gives an unadjusted-union $C_\alpha^0 = \bigcup_b C_\alpha^{[b]}$.
- For B even, an intermediate choice $\tau = 1/2$ amounts to constructing B single split confidence intervals at level $\alpha/2$, that is $C_{\alpha/2}^{[b]}$, which is a small but not negligible price to pay for using multiple splits rather than just one split. In practice, however, $\tau = 1/2$ and $C_\alpha^{[b]}$ may give marginal coverage $\approx 1 - \alpha$