Uncertainty Quantification for Machine Learning algorithms
An introduction to Conformal Prediction

Claire Boyer Margaux Zaffran

25-04-2023

MASPIN Days at FEMTO-ST

Machine learning context

Quantile Regression

Split Conformal Prediction (SCP)

Jackknife/cross-val

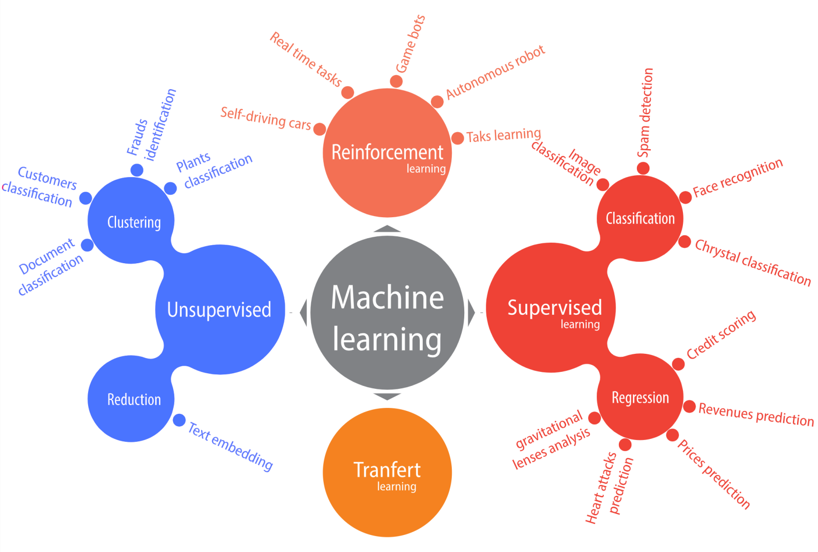
Distribution shift

Learning scenarios

ML develops generic methods for solving different types of problems:

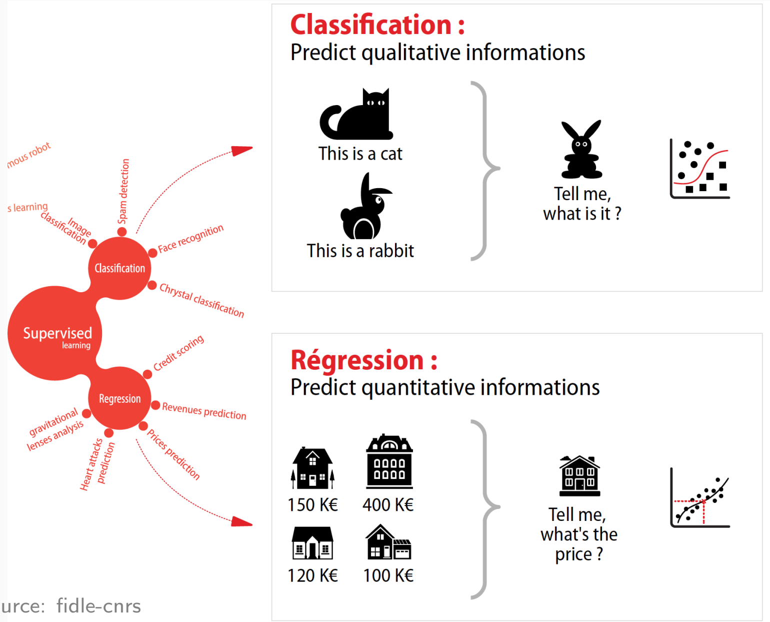
- Supervised learning
  Goal: learn from examples
- Unsupervised learning
  Goal: learn from data alone, extract structure in the data
- Reinforcement learning
  Goal: learn by exploring the environment (e.g. games or autonomous vehicle)

Learning scenarios



source: fidle-cnrs

Supervised learning



source: fidle-cnrs

Supervised learning, more formally

- Supervised learning: given a training sample $(X_i, Y_i)_{1 \leq i \leq n}$, the goal is to "learn" a predictor f_n such that

$$\underbrace{f_n(X_i) \simeq Y_i}_{\text{prediction on training data}} \qquad \text{and above all} \qquad \underbrace{f_n(X_{\text{new}}) \simeq Y_{\text{new}}}_{\text{prediction on test (unseen) data}}$$

  Often

- (classification) $X \in \mathbb{R}^d$ and $Y \in \{-1, 1\}$
- (regression) $X \in \mathbb{R}^d$ and $Y \in \mathbb{R}$

How to measure the performance of a predictor?

- Loss function in general: $\ell(Y, f(X))$ measures the goodness of the prediction of Y by $f(X)$
- Examples:
  - (classification) Prediction loss: $\ell(Y, f(X)) = \mathbf{1}_{Y \neq f(X)}$
  - (regression) Quadratic loss: $\ell(Y, f(X)) = |Y - f(X)|^2$
- The performance of a predictor f in regression is usually measured through the risk

$$\boxed{\mathrm{Risk}_\ell(f) = \mathbb{E}\Big[\ell\big(Y_{\mathrm{new}}, f(X_{\mathrm{new}})\big)\Big]}$$

- A minimizer $f^\star$ of the risk is called a Bayes predictor
  - (classification) $f^\star(X) = \mathrm{argmax}_k \mathbb{P}(Y = k|X)$
  - (regression) $f^\star(X) = \mathbb{E}[Y|X]$

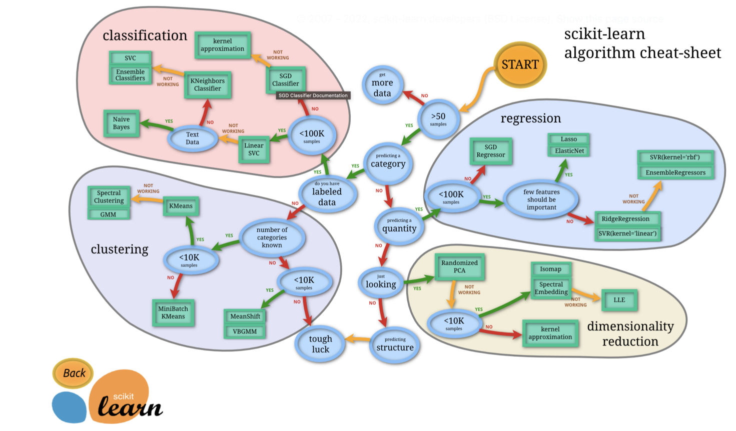
Learning by minimizing the empirical risk

- We want to construct a predictor with a small risk
- or an estimator of the Bayes predictor $f^\star$
- The distribution of the data is in general unknown, so is the risk
- Instead, given some training samples $(X_1, Y_1), \dots (X_n, Y_n)$, find the best predictor f that minimizes the empirical risk

$$\hat{\mathcal{R}}_n(f) := \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, f(X_i)).$$

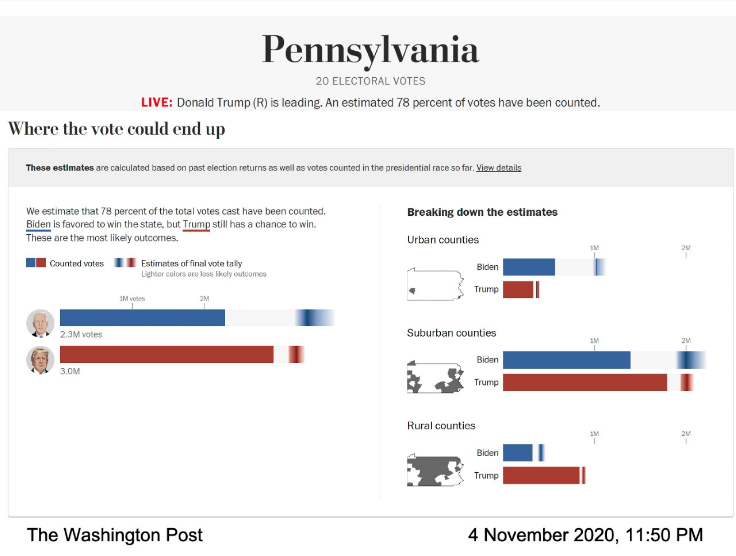
- Learning means retrieving information from training data by constructing a predictor that should have good performance on new data

There exist plenty of learners



see https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

On the importance of quantifying uncertainty



Machine learning context

Quantile Regression

Split Conformal Prediction (SCP)

Jackknife/cross-val

Distribution shift

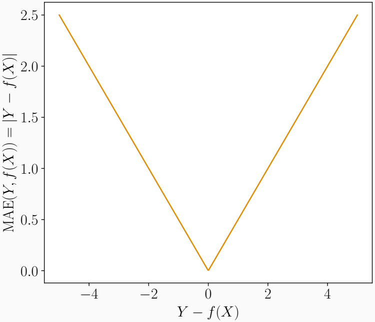
Reminder about quantiles

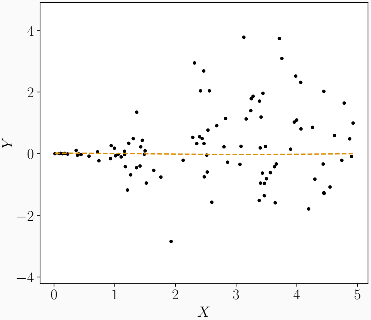
- **Quantile level** $\beta \in [0,1]$
- $Q_X(\beta) = \inf\{x \in \mathbb{R}^d, \mathbb{P}(X \leq x) \geq \beta\} = \inf\{x \in \mathbb{R}^d, F_X(x) \geq \beta\}$
- $q_\beta(X_1, \ldots, X_n) = \lceil \beta \times n \rceil -$ smallest value of $(X_1, \ldots, X_n)$

Median regression

- The Bayes predictor depends on the chosen loss function
- Mean Absolute Error (MAE) $\ell(Y, Y') = |Y - Y'|$
- Associated risk $\mathrm{Risk}_\ell(f) = \mathbb{E}\left[|Y - f(X)|\right]$
- Bayes predictor $f^\star \in \underset{f}{\operatorname{argmin}} \mathrm{Risk}_\ell(f)$

$$f^\star(X) = \mathrm{median}\left[Y|X\right] = Q_{Y|X}(0.5)$$





Generalization: Quantile regression

- Quantile level $\beta \in [0, 1]$
- Pinball loss

  $$\ell_\beta(Y, Y') = \beta|Y - Y'|\mathbb{1}_{\{|Y-Y'| \geq 0\}} + (1-\beta)|Y - Y'|\mathbb{1}_{\{|Y-Y'| \leq 0\}}$$
- Associated risk $\mathsf{Risk}_{\ell_\beta}(f) = \mathbb{E}\left[\ell_\beta(Y, f(X))\right]$
- Bayes predictor $f^\star \in \operatorname*{argmin}_f \mathsf{Risk}_{\ell_\beta}(f)$

  $$f^\star(X) = Q_{Y|X}(\beta)$$

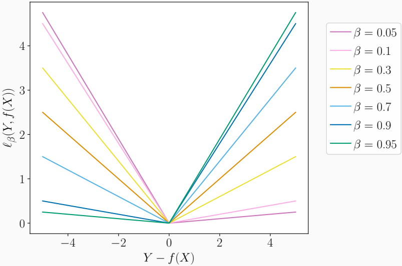
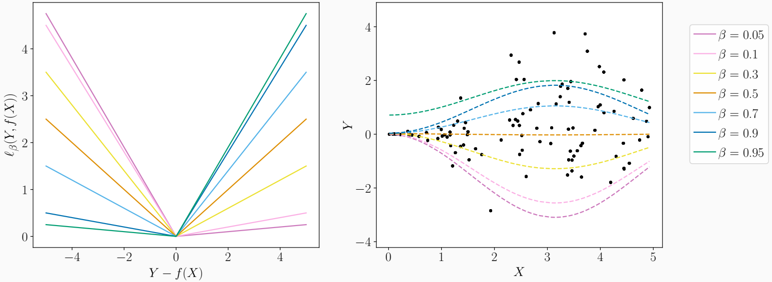


Figure 1: Pinball losses

Quantile regression



Warning

No theoretical guarantee with a finite sample

$$\mathbb{P}\left(Y \in \left[\hat{Q}_{Y|X}(\beta/2); \hat{Q}_{Y|X}(1-\beta/2)\right]\right) \neq 1 - \beta$$

Machine learning context

Quantile Regression

Split Conformal Prediction (SCP)

- Standard regression case
- Conformalized Quantile Regression (CQR)
- Generalization of SCP: going beyond regression

Jackknife/cross-val

Distribution shift

Quantifying predictive uncertainty

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- n training samples $(X_i, Y_i)_{i=1}^n$
- Goal: predict an unseen point Y_{n+1} at X_{n+1} with **confidence**
- How? Given a miscoverage level $\alpha \in [0, 1]$, build a predictive set $\mathcal{C}_\alpha$ such that:

$$\mathbb{P}\left\{Y_{n+1} \in \mathcal{C}_\alpha\left(X_{n+1}\right)\right\} \geq 1 - \alpha, \tag{1}$$

and $\mathcal{C}_\alpha$ should be as small as possible, in order to be informative.

SCP in regression

Training set	Calibration set	Test set

Algorithm

1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train your algorithm $\hat{A}$ on your proper training set
3. On the calibration set, get prediction values with $\hat{A}$
4. Obtain a set of $n_{\text{cal}} + 1$ conformity scores:

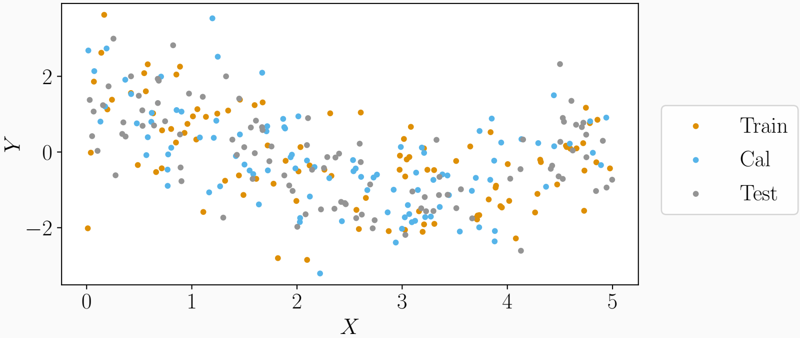
$$\mathcal{S} = \{S_i = |\hat{A}(X_i) - Y_i|, i \in \mathrm{Cal}\} \cup \{+\infty\}$$

(+ worst-case scenario)

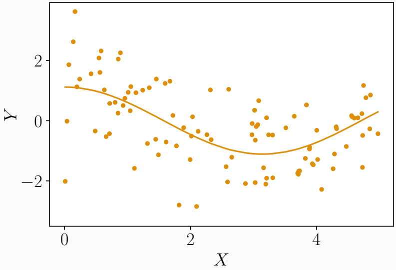
5. Compute the $1 - \alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
6. For a new point X_{n+1}, return

$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = \left[\hat{A}(X_{n+1}) - q_{1-\alpha}(\mathcal{S})\,;\,\hat{A}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})\right]$$

SCP in practice (splitting)

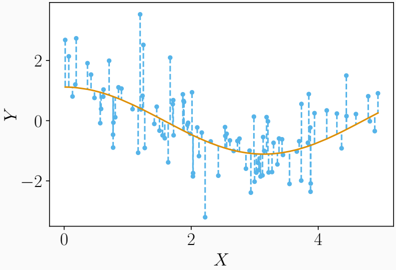


SCP in practice (training)



- Learn $\hat{\mu}$ on the training set

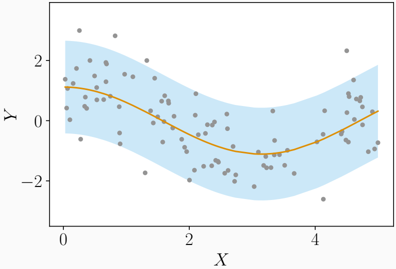
SCP in practice (calibration)



On the calibration set,

- Predict with $\hat{\mu}$
- Get the $|\text{residuals}|$
- Compute the $(1-\alpha)$ empirical quantile of the $|\text{residuals}| \cup \{+\infty\}$, noted $q_{1-\alpha}(\text{residuals})$

SCP in practice (prediction)



On the test set,

- Predict with $\hat{\mu}$
- Build $\widehat{\mathcal{C}}_\alpha(x)$:
  $[\hat{\mu}(x) \pm q_{1-\alpha}\,(\text{residuals})]$

SCP in theory

Definition (Exchangeability)

$(X_i, Y_i)_{i=1}^n$ are exchangeable if for any permutation σ of $[1, n]$ we have:

$$\mathcal{L}\left((X_1, Y_1), \ldots, (X_n, Y_n)\right) = \mathcal{L}\left(\left(X_{\sigma(1)}, Y_{\sigma(1)}\right), \ldots, \left(X_{\sigma(n)}, Y_{\sigma(n)}\right)\right),$$

where $\mathcal{L}$ designates the joint distribution.

Examples of exchangeable sequences

- i.i.d. samples
- Gaussian samples w/ expectation $m\mathbb{1}_d$ and covariance $\gamma^2 \mathrm{Id}_d + c\mathbb{1}_{d\times d}$

SCP in theory, cont'd

This procedure enjoys the finite sample guarantee proposed and proved in Vovk et al. (2005) and Lei et al. (2018).

Theorem

Suppose $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable (or i.i.d.). SCP applied on $(X_i, Y_i)_{i=1}^{n}$ outputs an interval $\widehat{\mathcal{C}}_\alpha(X_{n+1})$ such that:

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1})\right\} \geq 1 - \alpha.$$

If, in addition, the scores $\{S_i\}_{i \in \mathrm{Cal}}$ are almost surely distinct, then

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1})\right\} \leq 1 - \alpha + \frac{1}{n_{cal} + 1}.$$

✗ Marginal coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1}) \cancel{| X_{n+1} = x}\right\} \geq 1 - \alpha$

Proof architecture of SCP guarantees

Lemma (Quantile lemma)

If $(U_1, \dots, U_n, U_{n+1})$ *are exchangeable, then for any* $\beta \in]0,1[$*:*

$$\mathbb{P}\left(U_{n+1} \leq q_\beta(U_1, \dots, U_n, +\infty)\right) \geq \beta.$$

Additionally, if $U_1, \dots, U_n, U_{n+1}$ *are almost surely distinct, then:*

$$\mathbb{P}\left(U_{n+1} \leq q_\beta(U_1, \dots, U_n, +\infty)\right) \leq \beta + \frac{1}{n+1}.$$

Note that when $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable,

- the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ are exchangeable,
- therefore applying the quantile lemma to the scores concludes the proof.

Proof of the quantile lemma

$$U_{n+1} \leq q_\beta(U_1, \ldots, U_n, +\infty) \iff \frac{|\{i : U_i \leq U_{n+1}\}|}{n+1} \leq \beta$$

$$\iff \mathrm{rank}(U_{n+1}) \leq 1 + \beta(n+1)$$

Since $\mathrm{rank}(S_{n+1}) \sim \mathcal{U}(\{1, \ldots, n+1\})$, one gets

$$\mathbb{P}\left(\mathrm{rank}(U_{n+1}) \leq 1 + \beta(n+1)\right) = \frac{\lfloor 1 + \beta(n+1) \rfloor}{n+1}$$

$$\leq \frac{1 + \beta(n+1)}{n+1} = \beta + \frac{1}{n+1}$$

$$\geq \beta \qquad \text{(still true w/ ties)}$$

SCP: implementation details

Algorithm 1

1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train your algorithm $\hat{A}$ on your proper training set
3. On the calibration set, get prediction values with $\hat{A}$
4. Obtain a set of $n_{\text{cal}} + 1$ conformity scores:
$$\mathcal{S} = \{S_i = |\hat{A}(X_i) - Y_i|, i \in \mathrm{Cal}\} \cup \{+\infty\}$$
(+ worst-case scenario)
5. Compute the $1 - \alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
6. For a new point X_{n+1}, return
$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = [\hat{A}(X_{n+1}) - q_{1-\alpha}(\mathcal{S})\,;\, \hat{A}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$$

SCP: implementation details

Algorithm 2

Training set	Calibration set	Test set

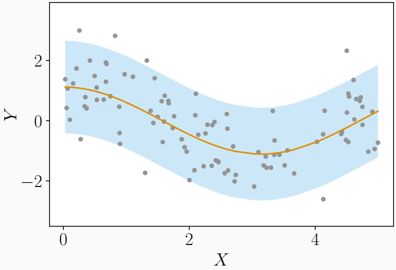
1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train your algorithm $\hat{A}$ on your proper training set
3. On the calibration set, get prediction values with $\hat{A}$
4. Obtain a set of n_{cal} conformity scores:

$$\mathcal{S} = \{S_i = |\hat{A}(X_i) - Y_i|, i \in \mathrm{Cal}\}$$

5. Compute the $(1-\alpha)\left(\frac{1}{n_{\text{cal}}} + 1\right)$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
6. For a new point X_{n+1}, return

$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = [\hat{A}(X_{n+1}) - q_{1-\alpha}(\mathcal{S})\,; \hat{A}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$$

Standard mean-regression SCP is not adaptive



On the test set,

- Predict with $\hat{\mu}$
- Build $\widehat{\mathcal{C}}_\alpha(x)$:
  $[\hat{\mu}(x) \pm q_{1-\alpha}(\text{residuals})]$

CQR (Romano et al., 2019)

Algorithm 1

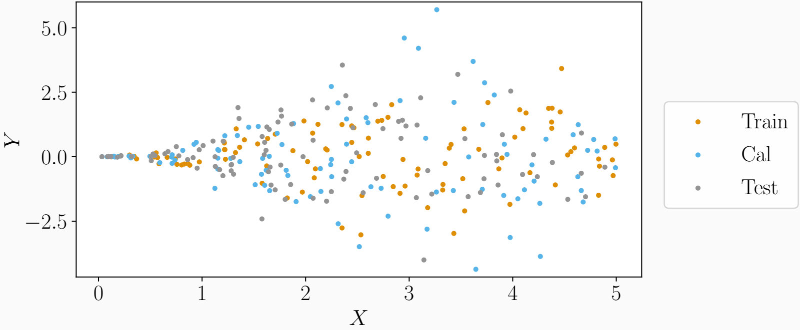
1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train two algorithms $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$ on the proper training set
3. Obtain a set of $n_{\text{cal}} + 1$ conformity scores $\mathcal{S}$:
   $\mathcal{S} = \{S_i = \max\left(\widehat{QR}_{\alpha/2}(X_i) - Y_i, Y_i - \widehat{QR}_{1-\alpha/2}(X_i)\right), i \in \mathrm{Cal}\} \cup \{+\infty\}$
4. Compute the $1-\alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
5. For a new point X_{n+1}, return
   $\widehat{\mathcal{C}}_\alpha(X_{n+1}) = [\widehat{QR}_{\alpha/2}(X_{n+1}) - q_{1-\alpha}(\mathcal{S})\,;\,\widehat{QR}_{1-\alpha/2}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$

CQR (Romano et al., 2019)

Algorithm 2

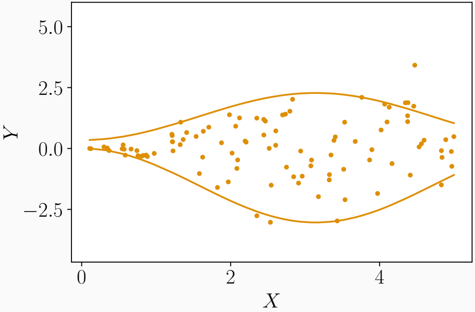
1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train two algorithms $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$ on the proper training set
3. Obtain a set of n_{cal} conformity scores $\mathcal{S}$:
   $\mathcal{S} = \{S_i = \max\left(\widehat{QR}_{\alpha/2}(X_i) - Y_i, Y_i - \widehat{QR}_{1-\alpha/2}(X_i)\right), i \in \mathrm{Cal}\} \cup \cancel{\{+\infty\}}$
4. Compute the $(1-\alpha)\left(\frac{1}{n_{\text{cal}}} + 1\right)$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
5. For a new point X_{n+1}, return
   $\widehat{\mathcal{C}}_\alpha(X_{n+1}) = [\widehat{QR}_{\alpha/2}(X_{n+1}) - q_{1-\alpha}(\mathcal{S})\,;\, \widehat{QR}_{1-\alpha/2}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$

CQR in practice



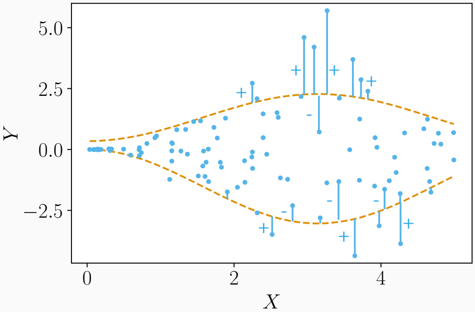
Randomly split the data to obtain a proper training set and a calibration set. Keep the test set.

CQR in practice (training)



- Learn $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$

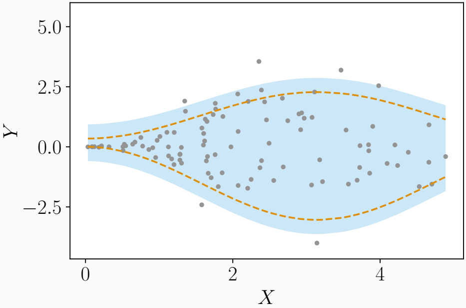
CQR in practice (calibration)



- Predict with $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$
- Compute the scores $\mathcal{S} = \{S_i\}_{\mathrm{Cal}} \cup \{+\infty\}$
- Get the $(1-\alpha)$ empirical quantile of the S_i, noted $q_{1-\alpha}(\mathcal{S})$

$$\hookrightarrow \quad S_i := \max\left\{ \widehat{QR}_{\alpha/2}(X_i) - Y_i, Y_i - \widehat{QR}_{1-\alpha/2}(X_i) \right\}$$

CQR in practice (prediction)



- Predict with $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$

- Build

$$\widehat{\mathcal{C}}_{\alpha}(x) = [\widehat{QR}_{\alpha/2}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{QR}_{1-\alpha/2}(x) + q_{1-\alpha}(\mathcal{S})]$$

CQR in theory

This procedure enjoys the finite sample guarantee proposed and proved in Romano et al. (2019).

Theorem

Suppose $(X_i, Y_i)_{i=1}^{n+1}$ *are exchangeable (or i.i.d.). CQR on* $(X_i, Y_i)_{i=1}^{n}$ *outputs* $\widehat{\mathcal{C}}_\alpha(X_{n+1})$ *such that:*

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1})\right\} \geq 1 - \alpha.$$

If, in addition, the scores $\{S_i\}_{i \in \mathrm{Cal}}$ *are almost surely distinct, then*

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1})\right\} \leq 1 - \alpha + \frac{1}{n_{cal} + 1}.$$

Proof: application of the quantile lemma.

✗ Marginal coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha(X_{n+1}) \cancel{| X_{n+1} = x}\right\} \geq 1 - \alpha$

SCP in general

1. Split randomly your training data into a proper training set (size n_{train}) and a calibration set (size n_{cal})
2. Train your algorithm $\hat{A}$ on your proper training set
3. On the calibration set, obtain $n_{\text{cal}} + 1$ conformity scores
   $\mathcal{S} = \{S_i = \text{s}(X_i, Y_i), i \in \text{Cal}\} \cup \{+\infty\}$

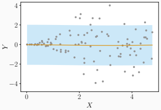
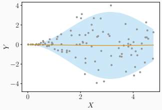
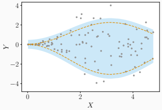
   Ex 1: $\text{s}(X_i, Y_i) = |\hat{A}(X_i) - Y_i|$ in regression with standard scores
   Ex 2: $\text{s}(X_i, Y_i) = \max\left(\widehat{QR}_{\alpha/2}(X_i) - Y_i, Y_i - \widehat{QR}_{1-\alpha/2}(X_i)\right)$ in CQR
4. Compute the $1 - \alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
5. For a new point X_{n+1}, return

$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = \{y \text{ such that } \text{s}(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\mathcal{S})\}$$

$\hookrightarrow$what is important is the definition of the conformity scores

SCP: what choices for the regression scores?

$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = \{y \text{ such that } \mathrm{s}(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\mathcal{S})\}$$

	Standard SCP Vovk et al. (2005)	**Locally weighted SCP** Lei et al. (2018)	**CQR** Romano et al. (2019)
$\mathrm{s}(X, Y)$	$\lvert\hat{A}(X) - Y\rvert$	$\frac{\lvert\hat{A}(X) - Y\rvert}{\hat{\rho}(X)}$	$\max(\widehat{QR}_{\alpha/2}(X) - Y,\ Y - \widehat{QR}_{1-\alpha/2}(X))$
$\widehat{\mathcal{C}}_\alpha(x)$	$\left[\hat{A}(x) \pm q_{1-\alpha}(\mathcal{S})\right]$	$\left[\hat{A}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)\right]$	$[\widehat{QR}_{\alpha/2}(x) - q_{1-\alpha}(\mathcal{S});\ \widehat{QR}_{1-\alpha/2}(x) + q_{1-\alpha}(\mathcal{S})]$
Visu.			
✓	black-box around a "usable" prediction	black-box around a "usable" prediction	adaptive
✗	not adaptive	limited adaptiveness	no black-box around a "usable" prediction

SCP in classification

- $Y_i \in \{1, \ldots, C\}$ (C classes)
- $\hat{A}(X) = (\hat{p}_1(X), \ldots, \hat{p}_C(X))$ (estimated probabilities)
- Score of the i-th calibration point: $S_i = 1 - (\hat{A}(X_i))_{Y_i}$
- For a new point X_{n+1}, return

$$\widehat{\mathcal{C}}_\alpha(X_{n+1}) = \{y \text{ such that } s(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\mathcal{S})\}$$

SCP in classification in practice

Ex: $Y_i \in \{$"dog", "tiger", "cat"$\}$, with $\alpha = 0.1$

- Scores on the calibration set

Cal_i	dog	dog	dog	tiger	tiger	tiger	tiger	cat	cat	cat
$\hat{p}_{\text{dog}}(X_i)$	0.95	0.90	0.85	0.15	0.15	0.20	0.15	0.15	0.25	0.20
$\hat{p}_{\text{tiger}}(X_i)$	0.02	0.05	0.10	0.60	0.55	0.50	0.45	0.40	0.35	0.45
$\hat{p}_{\text{cat}}(X_i)$	0.03	0.05	0.05	0.25	0.30	0.30	0.40	0.45	0.40	0.35
S_i	0.05	0.1	0.15	0.40	0.45	0.50	0.55	0.55	0.6	0.65

- $q_{1-\alpha}(\mathcal{S}) = 0.65$ $\quad\lceil 0.9 \times (10+1) \rceil = 10$
- $\hat{A}(X_{new}) = (0.05, 0.60, 0.35)$
  - $\hookrightarrow s(\hat{A}(X_{new}), \text{"dog"}) = 0.95$ $\quad$ "dog" $\notin \mathcal{C}_\alpha(X_{new})$
  - $\hookrightarrow s(\hat{A}(X_{new}), \text{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$ $\quad$ "tiger" $\in \mathcal{C}_\alpha(X_{new})$
  - $\hookrightarrow s(\hat{A}(X_{new}), \text{"cat"}) = 0.65 \leq q_{1-\alpha}(\mathcal{S})$ $\quad$ "cat" $\in \mathcal{C}_\alpha(X_{new})$
- $\mathcal{C}_\alpha(X_{new}) = \{$"tiger", "cat"$\}$

SCP in classification in practice

Ex: $Y_i \in \{$"dog", "tiger", "cat"$\}$, with $\alpha = 0.1$

- Scores on the calibration set

Cal_i	dog	dog	dog	tiger	tiger	tiger	tiger	cat	cat	cat
$\hat{p}_{\text{dog}}(X_i)$	0.95	0.90	0.85	0.05	0.05	0.05	0.05	0.10	0.10	0.15
$\hat{p}_{\text{tiger}}(X_i)$	0.02	0.05	0.10	0.85	0.80	0.75	0.70	0.25	0.30	0.30
$\hat{p}_{\text{cat}}(X_i)$	0.03	0.05	0.05	0.10	0.15	0.20	0.25	0.65	0.60	0.55
S_i	0.05	0.1	0.15	0.15	0.20	0.25	0.30	0.35	0.40	0.45

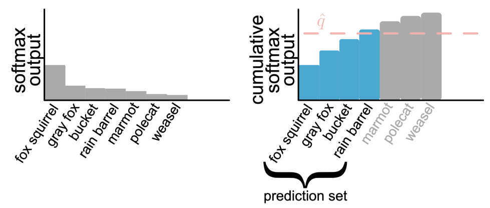
- $q_{1-\alpha}(\mathcal{S}) = 0.45$ $\qquad \lceil 0.9 \times (10+1) \rceil = 10$
- $\hat{A}(X_{new}) = (0.05, 0.60, 0.35)$
  - $\hookrightarrow$ $s(\hat{A}(X_{new}), \text{"dog"}) = 0.95$ $\qquad$ "dog" $\notin \mathcal{C}_\alpha(X_{new})$
  - $\hookrightarrow$ $s(\hat{A}(X_{new}), \text{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$ $\qquad$ "tiger" $\in \mathcal{C}_\alpha(X_{new})$
  - $\hookrightarrow$ $s(\hat{A}(X_{new}), \text{"cat"}) = 0.65$ $\qquad$ "cat" $\notin \mathcal{C}_\alpha(X_{new})$
- $\mathcal{C}_\alpha(X_{new}) = \{$"tiger"$\}$

SCP in classification: comments on the naive version

- Facts about the previous method
  - prediction sets with the smallest average size
  - undercover hard subgroups
  - overcover easy ones
- Other types of scores can be used to improve the conditional coverage (as in regression with CQR or localized)

SCP in classification: Adaptive Prediction Sets

1. Sort in decreasing order $\hat{p}_{\sigma_i(1)}(X_i) \geq \ldots \geq \hat{p}_{\sigma_i(C)}(X_i)$
2. $S_i = \sum_{k=1}^{\sigma_i^{-1}(Y_i)} \hat{p}_{\sigma_i(k)}(X_i)$ (sum of the estimated probabilities associated to classes at least as large as that of the true class Y_i)
3. Return the classes $\sigma_{\text{new}}(1), \ldots, \sigma_{\text{new}}(r^\star)$ where
$$r^\star = \arg\max_{1 \leq r \leq C} \left\{ \sum_{k=1}^{r} \hat{p}_{\sigma_{\text{new}}(k)}(X_{\text{new}}) < q_{1-\alpha}(\mathcal{S}) \right\} + 1$$



SCP in classification in practice: Adaptive Prediction Sets

Ex: $Y_i \in \{$"dog", "tiger", "cat"$\}$, with $\alpha = 0.1$

- Scores on the calibration set

Cal_i	dog	dog	dog	tiger	tiger	tiger	tiger	cat	cat	cat
$\hat{p}_{\text{dog}}(X_i)$	0.95	0.90	0.85	0.05	0.05	0.05	0.10	0.25	0.10	0.15
$\hat{p}_{\text{tiger}}(X_i)$	0.02	0.05	0.10	0.85	0.80	0.75	0.75	0.40	0.30	0.30
$\hat{p}_{\text{cat}}(X_i)$	0.03	0.05	0.05	0.10	0.15	0.20	0.15	0.35	0.60	0.55
S_i	0.95	0.90	0.85	0.85	0.80	0.75	0.75	0.75	0.60	0.55

- $q_{1-\alpha}(\mathcal{S}) = 0.95$
- Ex 1: $\hat{A}(X_{new}) = (0.05, 0.45, 0.5), r^\star = 2$

  $\mathcal{C}_\alpha(X_{new}) = \{$"tiger", "cat"$\}$
- Ex 2: $\hat{A}(X_{new}) = (0.03, 0.95, 0.02), r^\star = 1$

  $\mathcal{C}_\alpha(X_{new}) = \{$"tiger"$\}$

Split Conformal prediction: summary

- Simple procedure which
  - quantifies the uncertainty of a predictive model $\hat{A}$
  - by returning predictive regions
- Adapted to any predictive algorithm (neural nets, random forests...)
- Distribution-free as long as the data are exchangeable (and so are the scores)
- Finite-sample guarantees
- Marginal theoretical guarantee over the joint distribution of (X, Y), and not conditional, i.e., no guarantee that $\forall x \in \mathbb{R}$:

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{\mathcal{C}}_\alpha\left(X_{n+1}\right) \cancel{|X_{n+1} = x}\right\} \geq 1 - \alpha.$$

(despite some heuristics)

Challenges

- Conditional coverage (Previous Sec.)
- Computational cost vs. statistics power (Next Sec.: Jackknife)
- Exchangeability (Last Sec.: distribution shift)

Machine learning context

Quantile Regression

Split Conformal Prediction (SCP)

Jackknife/cross-val

Distribution shift

Full conformal prediction

Method: for a candidate (X_{new}, y),

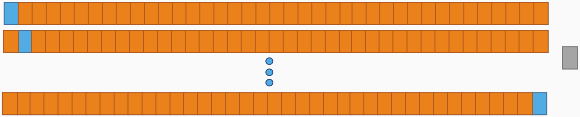
1. Train the algorithm $\hat{A}_y$ on $\{(X_1, Y_1), \dots, (X_n, Y_n)\} \cup \{(X_{\text{new}}, y)\}$
2. Scores
$$\mathcal{S}^{(\text{train})} = \left\{ s(\hat{A}_y(X_i), Y_i) \right\} \cup \{ s(\hat{A}_y(X_{\text{new}}), y) \}$$
3. $y \in \mathcal{C}_\alpha(X_{\text{new}})$ if $s(\hat{A}_y(X_{\text{new}}), y) \leq q_{1-\alpha}(\mathcal{S})$

✓ Theoretical guarantees (provided that $\hat{A}$ handles exchangeable training data in a symmetric way)

✗ Computationally costly: not used in practice

Jackknife: naive predictive interval

- Based on leave-one-out (LOO) residuals



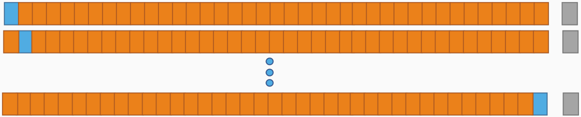
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
- Train $\hat{A}_{-i}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO scores $\mathcal{S} = \left\{ |\hat{A}_{-i}(X_i) - Y_i| \right\}_i \cup \{+\infty\}$ (in standard reg)
- Train $\hat{A}$ on $\mathcal{D}_n$
- Build the predictive interval: $\left[\hat{A}(X_{n+1}) \pm q_{1-\alpha}(\mathcal{S}) \right]$

Warning

No guarantee on the prediction of $\hat{A}$ with scores based on $(\hat{A}_{-i})_i$

Jackknife+ (Barber et al., 2021)

- Based on leave-one-out (LOO) residuals



- $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ training data
- Train $\hat{A}_{-i}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO predictions (in standard reg)
  $\mathcal{S}_{\text{up/down}} = \left\{ \hat{A}_{-i}(X_{n+1}) \pm |\hat{A}_{-i}(X_i) - Y_i| \right\}_i \cup \{\pm\infty\}$
- Build the predictive interval: $\left[q_{\alpha/2}(\mathcal{S}_{\text{down}}); q_{1-\alpha/2}(\mathcal{S}_{\text{up}}) \right]$

Theorem

If $\mathcal{D}_n \cup (X_{new}, Y_{new})$ are exchangeable and the algorithm treats the data points symmetrically, then $\mathbb{P}(Y_{new} \in \mathcal{C}_\alpha(X_{new})) \geq 1 - 2\alpha$.

- Based on cross-validation residuals
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data

1. Split $\mathcal{D}_n$ into K folds $F_1, \ldots, F_K$
2. Train $\hat{A}_{-F_k}$ on $\mathcal{D}_n \setminus F_k$
3. Cross-val predictions (in standard reg)
   $$\mathcal{S}_{\text{up/down}} = \left\{ \left\{ \hat{A}_{-F_k}(X_{n+1}) \pm |\hat{A}_{-F_k}(X_i) - Y_i| \right\}_{i \in F_k} \right\}_k \cup \{\pm\infty\}$$
4. Build the predictive interval: $[q_\alpha(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

Theorem

Under data exchangeability and algorithm symmetry, then
$$\mathbb{P}(Y_{new} \in \mathcal{C}_\alpha(X_{new})) \geq 1 - 2\alpha - \min\left(\frac{2(1-1/K)}{n/K+1}, \frac{1-K/n}{K+1}\right) \geq 1 - 2\alpha - \sqrt{2/n}.$$

Machine learning context

Quantile Regression

Split Conformal Prediction (SCP)

Jackknife/cross-val

Distribution shift

References i

Barber, R. F., Candès, E. J., Ramdas, A., and Tibshirani, R. J. (2021). Predictive inference with the jackknife+. *The Annals of Statistics*, 49(1):486–507.

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. J., and Wasserman, L. (2018). Distribution-Free Predictive Inference for Regression. *Journal of the American Statistical Association*.

Papadopoulos, H., Proedrou, K., Vovk, V., and Gammerman, A. (2002). Inductive Confidence Machines for Regression. In *Machine Learning: ECML 2002*. Springer.

Romano, Y., Patterson, E., and Candès, E. (2019). Conformalized Quantile Regression. *Advances in Neural Information Processing Systems*, 32.

References ii

Vovk, V., Gammerman, A., and Shafer, G. (2005). *Algorithmic Learning in a Random World*. Springer US.