Conformal Prediction: How to quantify uncertainty of machine learning models?

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ECAS-ENBIS course – ENBIS 2023 Annual conference

Presentation

- Last year statistics PhD Student, @ INRIA & École Polytechnique (Paris)
- Funded by Électricité de France *(French main electricity producer and supplier)*
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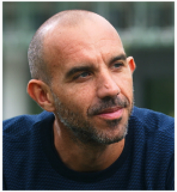

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- Research interests:
  - Distribution-free uncertainty quantification
  - Time series data
  - Missing values
  - Societal applications (energy, environmental and medical domains)

Supervised learning context and quantile regression

Split Conformal Prediction (SCP)

Avoiding data splitting: full conformal and out-of-bags approaches

Beyond exchangeability

Supervised learning setting

- **Data**: $(X_i, Y_i)_{i=1}^n \in \left(\mathbb{R}^d, \mathcal{Y}\right)^n$
- **Goal**: Learn a function $\hat{f}$ such that

$$\underbrace{i \in [\![1, n]\!] : \hat{f}(X_i) \simeq Y_i}_{\text{training data}} \quad \text{and moreover} \quad \underbrace{\hat{f}(X_{n+1}) \simeq Y_{n+1}}_{\text{prediction on test (unseen) data}}$$

- The supervised learning task is defined by the type of outcome:
  - $\mathcal{Y} = \{-1, 1\}$ $\longmapsto$ classification
  - $\mathcal{Y} = \mathbb{R}$ $\longmapsto$ regression

Supervised learning in theoretical practice

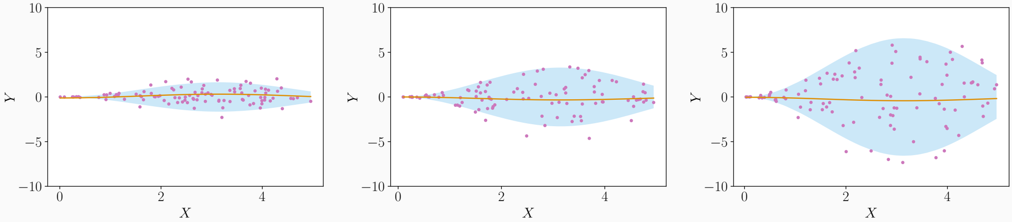
- **Loss function**: $\ell(Y, f(X))$ evaluates how close $f(X)$ is to Y
  - Classification $\rightsquigarrow$ 0-1 loss: $\ell(Y, f(X)) = \mathbf{1}_{Y \neq f(X)}$
  - Regression $\rightsquigarrow$ Quadratic loss: $\ell(Y, f(X)) = (Y - f(X))^2$
- $\hat{f}$ should be as good as possible over all the possible X:
  $\hookrightarrow$ focus on the **risk** of $\hat{f}$

$$\boxed{\mathrm{Risk}_\ell(f) = \mathbb{E}\Big[\ell\big(Y_{n+1}, f(X_{n+1})\big)\Big]}$$

- A minimizer $f^\star$ of the risk is called a Bayes predictor
  - Classification $\rightsquigarrow$ $f^\star(X) = \underset{k \in \{-1,1\}}{\operatorname{argmax}} \mathbb{P}(Y = k | X)$
  - Regression $\rightsquigarrow$ $f^\star(X) = \mathbb{E}[Y|X]$
- How to obtain $f^\star$ (i.e. minimize $\mathrm{Risk}_\ell(f)$) when the distribution of (X_{n+1}, Y_{n+1}) is unknown?
  $\hookrightarrow$ Minimize the empirical risk

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

On the importance of quantifying uncertainty



$\hookrightarrow$ Same predictions, yet 3 distinct underlying phenomena!

$\Longrightarrow$ Quantifying uncertainty conveys this information.

Reminder about quantiles

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

Example of quantile: the median

$\beta = 0.5$

$\hookrightarrow$ $q_{0.5}(X_1, \dots, X_n)$ is the empirical median of $(X_1, \dots, X_n)$;

$\hookrightarrow$ $Q_X(0.5)$ represents the median of the distribution of X.

Similarly, let $q_{\beta,\inf}(X_1, \dots, X_n) := \lfloor \beta \times n \rfloor$ smallest value of $(X_1, \dots, X_n)$

- The Bayes predictor depends on the chosen loss function.

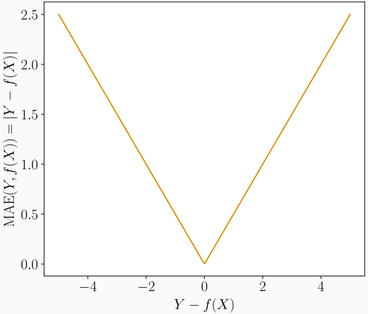
  $\hookrightarrow$ Bayes predictor $f^\star \in \operatorname*{argmin}_f \mathsf{Risk}_\ell(f)$

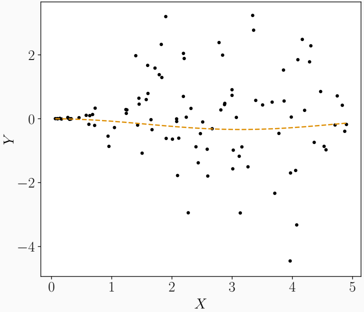
$$:= \operatorname*{argmin}_f \mathbb{E}\left[\ell(Y, f(X))\right]$$

- Mean Absolute Error (MAE): $\ell(Y, Y') = |Y - Y'|$

  Associated risk: $\mathsf{Risk}_\ell(f) = \mathbb{E}\left[|Y - f(X)|\right]$

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





Generalization: Quantile regression

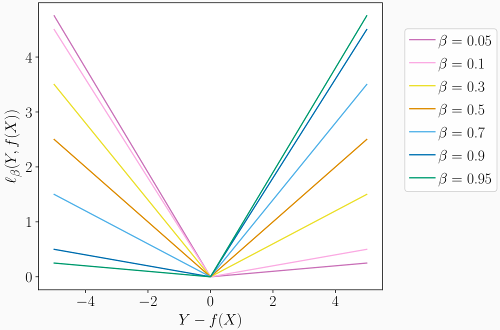
- Quantile level $\beta \in [0, 1]$
- Pinball loss

$$\ell_\beta(Y, Y') = \beta |Y - Y'| \mathbb{1}_{\{|Y - Y'| \geq 0\}} + (1 - \beta) |Y - Y'| \mathbb{1}_{\{|Y - Y'| \leq 0\}}$$

Associated risk: $\text{Risk}_{\ell_\beta}(f) = \mathbb{E}\left[\ell_\beta(Y, f(X))\right]$

Bayes predictor: $f^\star \in \operatorname*{argmin}_f \text{Risk}_{\ell_\beta}(f)$

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

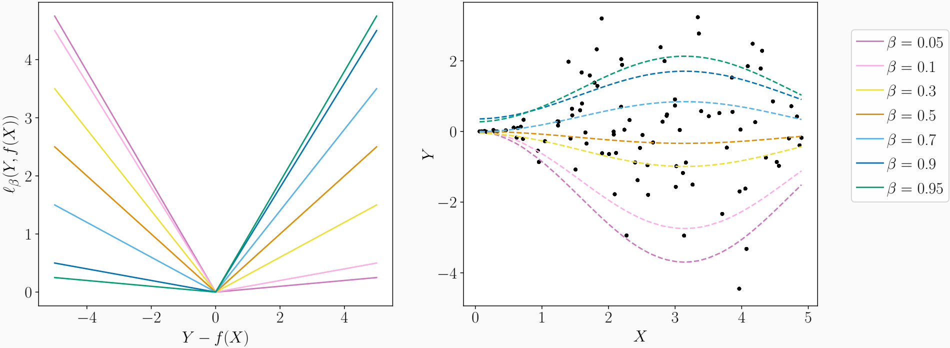


Quantile regression: foundations

- Link between the pinball loss and the quantiles?
  Set $q^\star \in \arg\min_q \mathbb{E}\left[\ell_\beta(Y - q)\right]$. Then,

$$
\begin{aligned}
0 &= \int_{-\infty}^{+\infty} \ell'_\beta(y - q^\star) df_Y(y) \\
&= (\beta - 1)\int_{-\infty}^{q^\star} df_Y(y) + \beta \int_{q^\star}^{+\infty} df_Y(y) \\
0 &= (\beta - 1)F_Y(q^\star) + \beta(1 - F_Y(q^\star)) \\
(1-\beta)F_Y(q^\star) &= \beta(1 - F_Y(q^\star)) \\
\beta &= F_Y(q^\star) \\
\Leftrightarrow q^\star &= F_Y^{-1}(\beta)
\end{aligned}
$$

Quantile regression: visualisation



Warning

No theoretical guarantee with a finite sample!

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

Supervised learning context and quantile regression

Split Conformal Prediction (SCP)

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

Avoiding data splitting: full conformal and out-of-bags approaches

Beyond exchangeability

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

  For example: $\alpha = 0.1$ and obtain a 90% coverage interval
- Construction of the predictive intervals should be
  - agnostic to the model
  - agnostic to the data distribution
  - valid in finite samples

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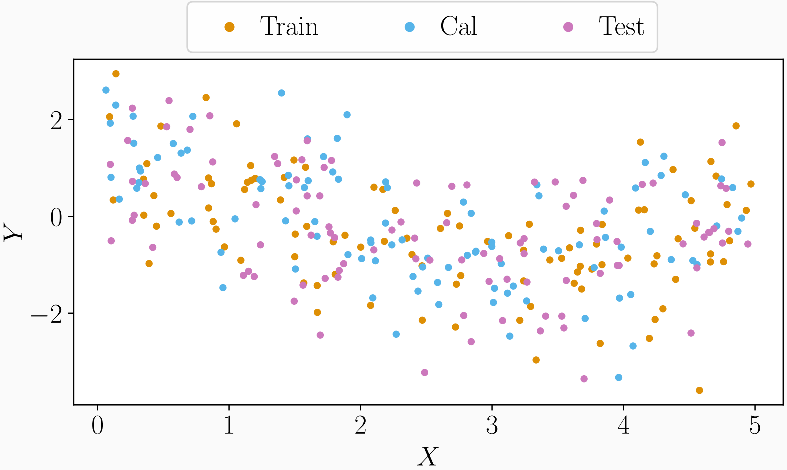
Split Conformal Prediction (SCP)[1,2,3]: toy example

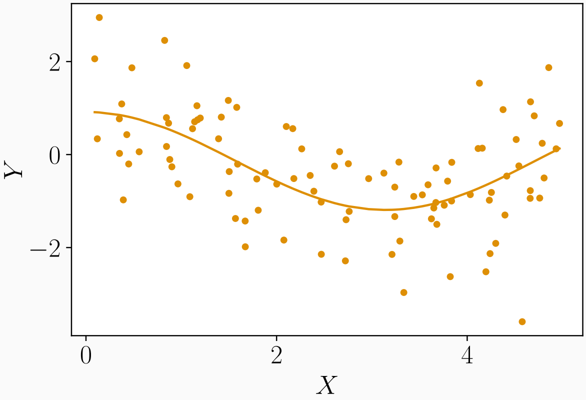


[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*

[2] Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML

[3] Lei et al. (2018), *Distribution-Free Predictive Inference for Regression*, JRSS B

Split Conformal Prediction (SCP)[1,2,3]: training step



- Learn (or get) $\hat{\mu}$

[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*
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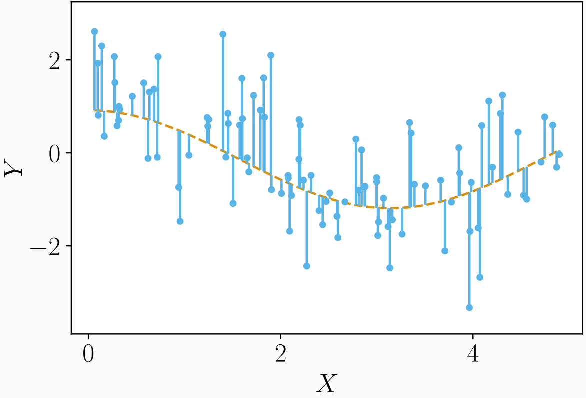
Split Conformal Prediction (SCP)[1,2,3]: calibration step



- Predict with $\hat{\mu}$
- Get the $|\text{residuals}|$, a.k.a. conformity scores
- Compute the $(1-\alpha)$ empirical quantile of $\mathcal{S} = \{|\text{residuals}|\}_{\text{Cal}} \cup \{+\infty\}$, noted $q_{1-\alpha}(\mathcal{S})$

[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*
[2] Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML
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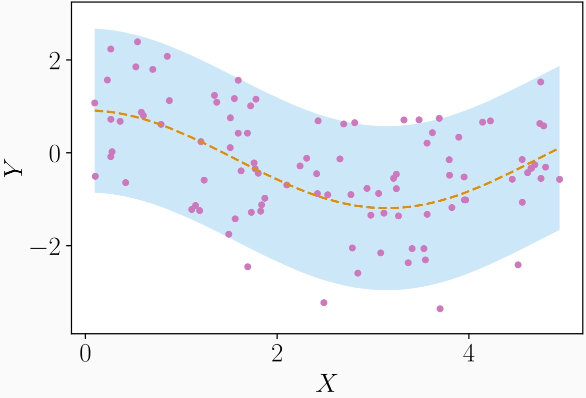
Split Conformal Prediction (SCP)[1,2,3]: prediction step



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

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[2] Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML
[3] Lei et al. (2018), *Distribution-Free Predictive Inference for Regression*, JRSS B

SCP: implementation details

1. Randomly split the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
2. Get $\hat{\mu}$ *by training the algorithm* $\mathcal{A}$ *on the proper training set*
3. On the calibration set, get prediction values with $\hat{\mu}$
4. Obtain a set of $\#\mathrm{Cal}+1$ conformity scores:

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

(+ 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

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

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SCP: theoretical foundation

Definition (Exchangeability)

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

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

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

Examples of exchangeable sequences

- i.i.d. samples
- The components of $\mathcal{N}\left(\begin{pmatrix} m \\ \vdots \\ \vdots \\ m \end{pmatrix}, \begin{pmatrix} \sigma^2 & & & \\ & \ddots & \gamma^2 & \\ & \gamma^2 & \ddots & \\ & & & \sigma^2 \end{pmatrix}\right)$

SCP: theoretical guarantees

SCP enjoys finite sample guarantees proved in Vovk et al. (2005); Lei et al. (2018).

Theorem

Suppose $(X_i, Y_i)_{i=1}^{n+1}$ *are exchangeable*[4]. *SCP applied on* $(X_i, Y_i)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha(\cdot)$ *such that:*

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

Additionally, if the scores $\{S_i\}_{i \in \mathrm{Cal}}$ *are a.s. distinct:*

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

[4] Only the calibration and test data need to be exchangeable.

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:

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

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.
$\hookrightarrow$ applying the quantile lemma to the scores concludes the proof.

Proof of the quantile lemma

First note that $U_{n+1} \leq q_\beta(U_1, \dots, U_n, +\infty) \iff U_{n+1} \leq q_\beta(U_1, \dots, U_n, U_{n+1})$.

Then, by definition of q_β:

$$U_{n+1} \leq q_\beta(U_1, \dots, U_n, U_{n+1}) \iff \mathrm{rank}(U_{n+1}) \leq \lceil \beta(n+1) \rceil$$

By exchangeability, $\mathrm{rank}(U_{n+1}) \sim \mathcal{U}\{1, \dots, n+1\}$. Thus:

$$\mathbb{P}\left(\mathrm{rank}(U_{n+1}) \leq \lceil \beta(n+1) \rceil\right) \geq \frac{\lceil \beta(n+1) \rceil}{n+1} \geq \beta.$$

If $U_1, \dots, U_n, U_{n+1}$ are almost surely distinct (without ties):

$$\begin{aligned}
\mathbb{P}\left(\mathrm{rank}(U_{n+1}) \leq \lceil \beta(n+1) \rceil\right) &= \frac{\lceil \beta(n+1) \rceil}{n+1} \\
&\leq \frac{1 + \beta(n+1)}{n+1} = \beta + \frac{1}{n+1}.
\end{aligned}$$

$\square$

SCP: theoretical guarantees

SCP enjoys finite sample guarantees proved in Vovk et al. (2005); Lei et al. (2018).

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Additionally, if the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ *are a.s. distinct:*

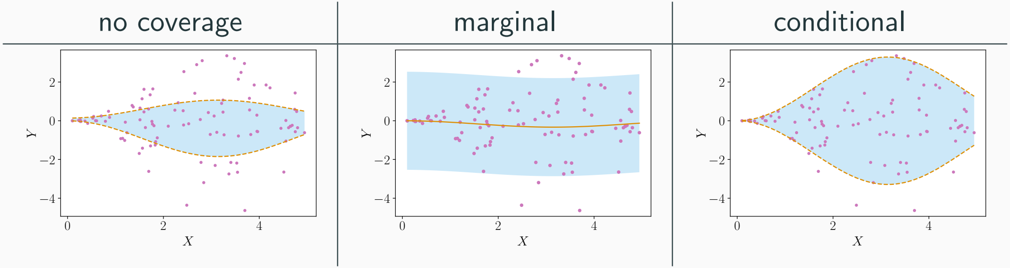
$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})\right\} \leq 1 - \alpha + \frac{1}{\#\mathrm{Cal} + 1}.$$

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

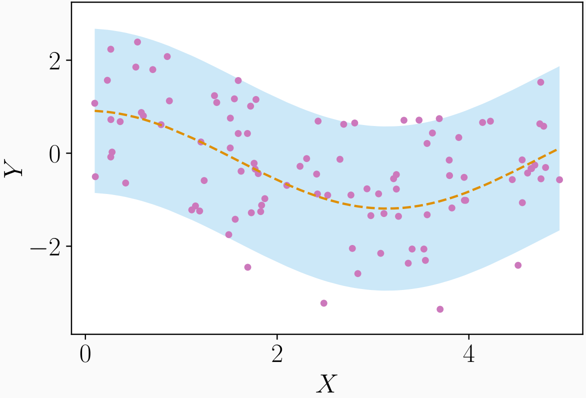
[4] Only the calibration and test data need to be exchangeable.

Conditional coverage implies adaptiveness

- Marginal coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha\left(X_{n+1}\right)\right\}$ the errors may differ across regions of the input space (i.e. non-adaptive)
- Conditional coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha\left(X_{n+1}\right) \middle| X_{n+1}\right\}$ errors are evenly distributed (i.e. fully adaptive)
- Conditional coverage is stronger than marginal coverage



Standard mean-regression SCP is not adaptive



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

Informative conditional coverage as such is impossible

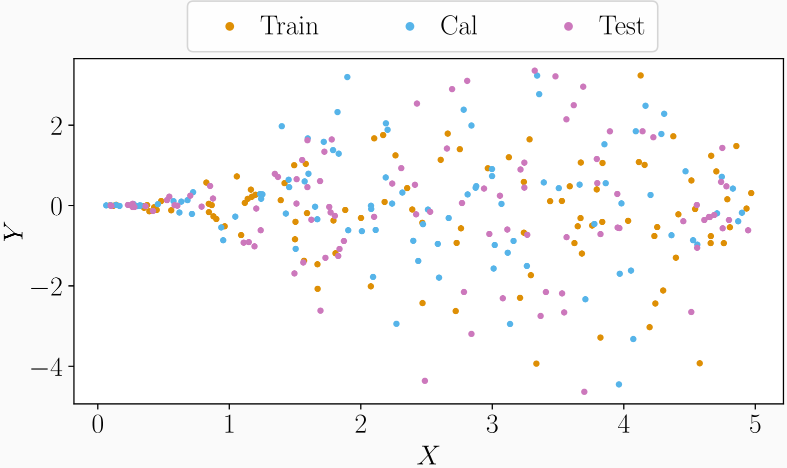
- Impossibility results
  $\hookrightarrow$ Lei and Wasserman (2014); Vovk (2012); Barber et al. (2021a)

> Without distribution assumption, in finite sample, a perfectly conditionally valid $\widehat{C}_\alpha$ is such that $\mathbb{P}\left\{\text{mes}\left(\widehat{C}_\alpha(x)\right) = \infty\right\} = 1$ for any non-atomic x.

- Approximate conditional coverage
  $\hookrightarrow$ Romano et al. (2020a); Guan (2022); Jung et al. (2023); Gibbs et al. (2023)
  Target $\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha | X_{n+1} \in \mathcal{R}(x)) \geq 1 - \alpha$
- Asymptotic (with the sample size) conditional coverage
  $\hookrightarrow$ Romano et al. (2019); Kivaranovic et al. (2020); Chernozhukov et al. (2021); Sesia and Romano (2021); Izbicki et al. (2022)

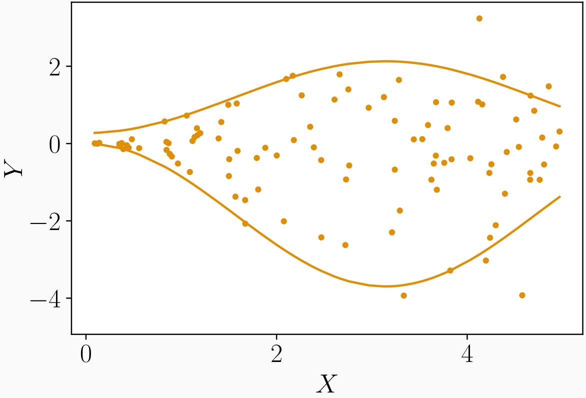
Non exhaustive references.

Conformalized Quantile Regression (CQR)[5]



[5] Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

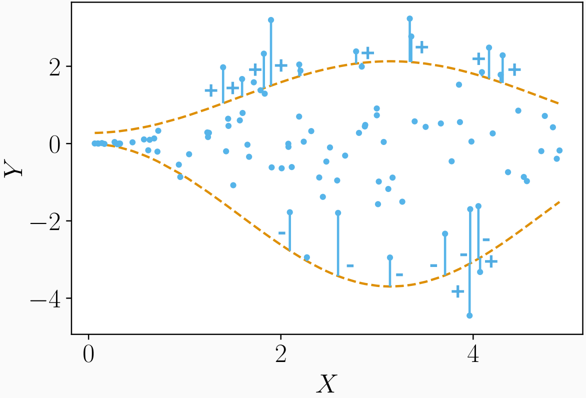
Conformalized Quantile Regression (CQR)[5]: training step



- Learn (or get) $\widehat{\mathrm{QR}}_{\mathrm{lower}}$ and $\widehat{\mathrm{QR}}_{\mathrm{upper}}$

[5] Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

Conformalized Quantile Regression (CQR)[5]: calibration step

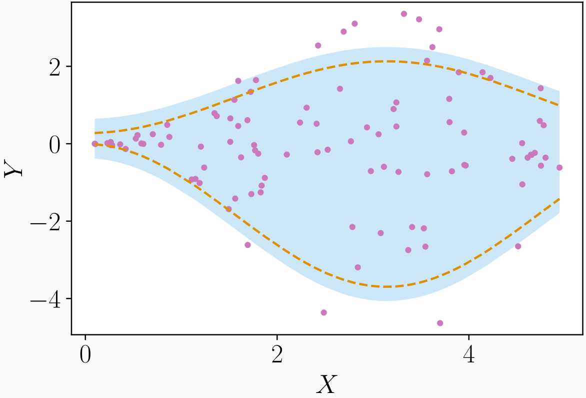


- Predict with $\widehat{\mathrm{QR}}_{\mathrm{lower}}$ and $\widehat{\mathrm{QR}}_{\mathrm{upper}}$
- Get the scores $\mathcal{S} = \{S_i\}_{\mathrm{Cal}} \cup \{+\infty\}$
- Compute the $(1-\alpha)$ empirical quantile of $\mathcal{S}$, noted $q_{1-\alpha}(\mathcal{S})$

$$\hookrightarrow \quad S_i := \max\left\{\widehat{\mathrm{QR}}_{\mathrm{lower}}(X_i) - Y_i, Y_i - \widehat{\mathrm{QR}}_{\mathrm{upper}}(X_i)\right\}$$

[5] Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

Conformalized Quantile Regression (CQR)[5]: prediction step



- Predict with $\widehat{\text{QR}}_{\text{lower}}$ and $\widehat{\text{QR}}_{\text{upper}}$

- Build

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

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CQR: implementation details

1. Randomly split the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
2. Get $\widehat{\mathrm{QR}}_{\mathrm{lower}}$ and $\widehat{\mathrm{QR}}_{\mathrm{upper}}$ *by training the algorithm $\mathcal{A}$ on the proper training set*
3. Obtain a set of $\#\mathrm{Cal}+1$ conformity scores $\mathcal{S}$:
$$\mathcal{S} = \{S_i = \max\left(\widehat{\mathrm{QR}}_{\mathrm{lower}}(X_i) - Y_i, Y_i - \widehat{\mathrm{QR}}_{\mathrm{upper}}(X_i)\right), i \in \mathrm{Cal}\} \cup \{+\infty\}$$
4. Compute the $1-\alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
5. For a new point X_{n+1}, return
$$\widehat{C}_\alpha(X_{n+1}) = [\widehat{\mathrm{QR}}_{\mathrm{lower}}(X_{n+1}) - q_{1-\alpha}(\mathcal{S}); \widehat{\mathrm{QR}}_{\mathrm{upper}}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$$

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CQR: theoretical guarantees

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*[6]. *CQR on* $(X_i, Y_i)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha(\cdot)$ *such that:*

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

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

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

Proof: application of the quantile lemma.

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

[6] Only the calibration and test data need to be exchangeable.

SCP is defined by the conformity score function

1. Randomly split the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
2. Get $\hat{A}$ *by training the algorithm $\mathcal{A}$ on the proper training set*
3. On the calibration set, obtain $\#\mathrm{Cal}+1$ conformity scores

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

   Ex 1: $\mathrm{s}(\hat{A}(X_i), Y_i) := |\hat{\mu}(X_i) - Y_i|$ in regression with standard scores

   Ex 2: $\mathrm{s}(\hat{A}(X_i), Y_i) := \max\left(\widehat{\mathrm{QR}}_{\text{lower}}(X_i) - Y_i, Y_i - \widehat{\mathrm{QR}}_{\text{upper}}(X_i)\right)$ in CQR

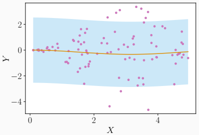
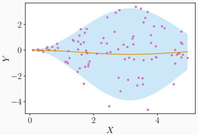
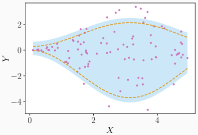
4. Compute the $1-\alpha$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
5. For a new point X_{n+1}, return

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

$\hookrightarrow$ The definition of the conformity scores is crucial, as they incorporate almost all the information: data + underlying model

SCP: what choices for the regression scores?

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

	Standard SCP Vovk et al. (2005)	**Locally weighted SCP** Lei et al. (2018)	**CQR** Romano et al. (2019)
$\mathrm{s}(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$	$\frac{\lvert\hat{\mu}(X) - Y\rvert}{\hat{\rho}(X)}$	$\max(\widehat{\mathrm{QR}}_{\text{lower}}(X) - Y, Y - \widehat{\mathrm{QR}}_{\text{upper}}(X))$
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)]$	$[\widehat{\mathrm{QR}}_{\text{lower}}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{\mathrm{QR}}_{\text{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
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: theoretical guarantees

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

Theorem

Suppose $(X_i, Y_i)_{i=1}^{n+1}$ *are exchangeable*[7]*. SCP on* $(X_i, Y_i)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha(\cdot)$ *such that:*

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

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

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

Proof: application of the quantile lemma.

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

[7] Only the calibration and test data need to be exchangeable.

SCP: standard classification

- $Y \in \{1, \dots, C\}$ (C classes)
- $\hat{A}(X) = (\hat{p}_1(X), \dots, \hat{p}_C(X))$ (estimated probabilities)
- $\mathsf{s}(\hat{A}(X), Y) := 1 - (\hat{A}(X))_Y$
- For a new point X_{n+1}, return

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

SCP: standard classification in practice

Ex: $Y_i \in \{\text{"dog"}, \text{"tiger"}, \text{"cat"}\}$, 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

- $q_{1-\alpha}(\mathcal{S}) = 0.65$
- $\hat{A}(X_{n+1}) = (\mathbf{0.05}, \mathbf{0.60}, \mathbf{0.35})$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \textbf{"dog"}) = 0.95$ $\qquad$ "dog" $\notin \widehat{C}_\alpha(X_{n+1})$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \textbf{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$ $\qquad$ "tiger" $\in \widehat{C}_\alpha(X_{n+1})$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \textbf{"cat"}) = 0.65 \leq q_{1-\alpha}(\mathcal{S})$ $\qquad$ "cat" $\in \widehat{C}_\alpha(X_{n+1})$
- $\widehat{C}_\alpha(X_{n+1}) = \{\text{"tiger"}, \text{"cat"}\}$

SCP: standard classification in practice, cont'd

Ex: $Y \in \{$"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

- $q_{1-\alpha}(\mathcal{S}) = 0.45$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \text{"dog"}) = 0.95$ — "dog" $\notin \widehat{C}_\alpha(X_{n+1})$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \text{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$ — "tiger" $\in \widehat{C}_\alpha(X_{n+1})$
  - $\hookrightarrow$ $\mathrm{s}(\hat{A}(X_{n+1}), \text{"cat"}) = 0.65$ — "cat" $\notin \widehat{C}_\alpha(X_{n+1})$
- $\widehat{C}_\alpha(X_{n+1}) = \{$"tiger"$\}$

SCP: limits of the standard classification case

The standard classification conformity score function leads to:

- ✓ smallest prediction sets on average
- ✗ undercovering (overcovering) hard (easy) subgroups

(similar to the standard mean regression case!)

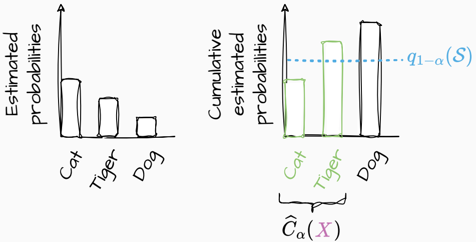
$\Rightarrow$ Other score functions can be built to improve adaptiveness

(as in regression with localized scores)

SCP: classification with Adaptive Prediction Sets[8]

1. Sort in decreasing order $\hat{p}_{\sigma(1)}(X) \geq \ldots \geq \hat{p}_{\sigma(C)}(X)$
2. $s(\hat{A}(X), Y) := \sum_{k=1}^{\sigma^{-1}(Y)} \hat{p}_{\sigma(k)}(X)$ (sum of the estimated probabilities associated to classes at least as large as that of the true class Y)
3. Return the set of classes $\{\sigma_{n+1}(1), \ldots, \sigma_{n+1}(r^\star)\}$, where

$$r^\star = \underset{1 \leq r \leq C}{\arg\max} \left\{ \sum_{k=1}^{r} \hat{p}_{\sigma_{n+1}(k)}(X_{n+1}) < q_{1-\alpha}(\mathcal{S}) \right\} + 1$$



[8] Romano et al. (2020b), *Classification with Valid and Adaptive Coverage*, NeurIPS
Figure highly inspired by Angelopoulos and Bates (2023).

SCP: classification with Adaptive Prediction Sets in practice

Ex: $Y \in \{$"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

- $q_{1-\alpha}(\mathcal{S}) = 0.95$

$\hookrightarrow$ Ex 1: $\hat{A}(X_{n+1}) = (0.05, 0.45, 0.5)$, $r^\star = 2$

$\widehat{C}_\alpha(X_{n+1}) = \{$"tiger", "cat"$\}$

$\hookrightarrow$ Ex 2: $\hat{A}(X_{n+1}) = (0.03, 0.95, 0.02)$, $r^\star = 1$

$\widehat{C}_\alpha(X_{n+1}) = \{$"tiger"$\}$

Split Conformal Prediction: summary

- **Simple** procedure which quantifies the uncertainty of **any** predictive model $\hat{A}$ by returning predictive regions
- **Finite-sample** guarantees
- **Distribution-free** as long as the data are exchangeable (and so are the scores)
- **Marginal** theoretical guarantee over the joint (X, Y) distribution, and not conditional, i.e., no guarantee that for any x:

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

$\hookrightarrow$ marginal also over the whole calibration set and the test point!

Challenges: open questions (non exhaustive!)

- Conditional coverage (~ Previous Section)
- Computational cost vs statistical power (Next Section)
- Exchangeability (Last Section)

Supervised learning context and quantile regression

Split Conformal Prediction (SCP)

Avoiding data splitting: full conformal and out-of-bags approaches

- Full Conformal Prediction
- Jackknife+

Beyond exchangeability

Supervised learning context and quantile regression

Split Conformal Prediction (SCP)

Avoiding data splitting: full conformal and out-of-bags approaches

Full Conformal Prediction

Jackknife+

Beyond exchangeability

Splitting the data might not be desired

SCP suffers from data splitting:

- lower statistical efficiency (lower model accuracy and higher predictive set size)
- higher statistical variability

Can we avoid splitting the data set?

The naive idea does not enjoy valid coverage (even empirically)

- A naive idea:
    - Get $\hat{A}$ by training the algorithm $\mathcal{A}$ on $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$.
    - compute the empirical quantile $q_{1-\alpha}(\mathcal{S})$ of the set of scores

$$\mathcal{S} = \left\{ \mathrm{s}\left(\hat{A}\left(X_i\right), Y_i\right) \right\}_{i=1}^{n} \cup \{\infty\}.$$

    - output the set $\left\{ y \text{ such that } \mathrm{s}\left(\hat{A}\left(X_{n+1}\right), y\right) \leq q_{1-\alpha}(\mathcal{S}) \right\}$.

✗ $\hat{A}$ has been obtained using the training set $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ but did not use X_{n+1}.
$\Rightarrow \mathrm{s}\left(\hat{A}\left(X_{n+1}\right), y\right)$ stochastically dominates any element of $\left\{ \mathrm{s}\left(\hat{A}\left(X_i\right), Y_i\right) \right\}_{i=1}^{n}$.

Full Conformal Prediction[9] does not discard training points!

- Full *(or transductive)* Conformal Prediction
  - avoids data splitting
  - at the cost of many more model fits
- **Idea**: the most probable labels Y_{n+1} live in $\mathcal{Y}$, and have a low enough conformity score. By looping over all possible $y \in \mathcal{Y}$, the ones leading to the smallest conformity scores will be found.

[9] Vovk et al. (2005), *Algorithmic Learning in a Random World*

Full Conformal Prediction (CP): recovering exchangeability

For any candidate (X_{n+1}, y),

1. Get $\hat{A}_y$ by training $\mathcal{A}$ on $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \cup \{(X_{n+1}, y)\}$
2. Obtain a set of training scores
$$\mathcal{S}^{(\text{train})} = \left\{ \boxed{\mathrm{s}}(\hat{A}_y(X_i), Y_i) \right\}_{i=1}^{n} \cup \{ \boxed{\mathrm{s}}(\hat{A}_y(X_{n+1}), y)\}$$
   and compute their $1 - \alpha$ empirical quantile $q_{1-\alpha}\left(\mathcal{S}^{(\text{train})}\right)$
3. Output the set $\left\{ y \text{ such that } \boxed{\mathrm{s}}\left(\hat{A}_y\left(X_{n+1}\right), y\right) \le q_{1-\alpha}\left(\mathcal{S}^{(\text{train})}\right) \right\}$

✓ Test point treated in the same way than train points

✗ Computationally costly

Full CP: theoretical foundation

Definition (Symmetrical algorithm)

A deterministic algorithm $\mathcal{A} : (U_1, \ldots, U_n) \mapsto \hat{A}$ is symmetric if for any permutation σ of $[\![1, n]\!]$:

$$\mathcal{A}\left(U_1, \ldots, U_n\right) \overset{\text{a.s.}}{=} \mathcal{A}\left(U_{\sigma(1)}, \ldots, U_{\sigma(n)}\right).$$

Full CP: theoretical guarantees

Full CP enjoys finite sample guarantees proved in Vovk et al. (2005).

Theorem

Suppose that

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

(ii) *the algorithm* $\mathcal{A}$ *is symmetric.*

Full CP applied on $(X_i, Y_i)_{i=1}^{n} \cup \{X_{n+1}\}$ *outputs* $\widehat{C}_\alpha(\cdot)$ *such that:*

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

Additionally, if the scores are a.s. distinct:

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

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

FCP sets with an interpolating algorithm

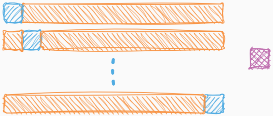
Assume $\mathcal{A}$ interpolates:

- $\hat{A} = \mathcal{A}\left((x_1, y_1), \ldots, (x_{n+1}, y_{n+1})\right)$
- $\hat{A}(x_k) - y_k = 0$ for any $k \in [\![1, n+1]\!]$

$\Rightarrow$ Full Conformal Prediction outputs $\mathcal{Y}$ (the whole label space) for any new test point!

Jackknife: the naive idea does not enjoy valid coverage

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



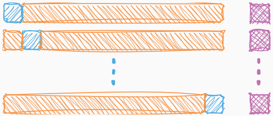
- $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO scores $\mathcal{S} = \left\{ |\hat{A}_{-i}(X_i) - Y_i| \right\}_i \cup \{+\infty\}$ (in standard mean regression)
- Get $\hat{A}$ by training $\mathcal{A}$ 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 $(\hat{A}_{-i})_i$, without assuming a form of **stability** on $\mathcal{A}$.

Jackknife+[10]

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



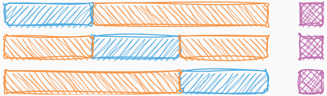
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO predictions / predictive intervals
  $\mathcal{S}_{\text{up/down}} = \left\{ \hat{A}_{-i}(X_{n+1}) \pm |\hat{A}_{-i}(X_i) - Y_i| \right\}_i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

Theorem

If $\mathcal{D}_n \cup (X_{n+1}, Y_{n+1})$ are exchangeable and $\mathcal{A}$ is symmetric: $\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})) \geq 1 - 2\alpha$.

[10] Barber et al. (2021b), *Predictive Inference with the jackknife+*, The Annals of Statistics
Recall $q_{\beta,\inf}(X_1, \ldots, X_n) := \lfloor \beta \times n \rfloor$ smallest value of $(X_1, \ldots, X_n)$

CV+ [11] (see also cross-conformal predictors: Vovk, 2015)



- Based on cross-validation residuals
- $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ training data
- Split $\mathcal{D}_n$ into K folds $F_1, \dots, F_K$
- Get $\hat{A}_{-F_k}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus F_k$
- Cross-val predictions / predictive intervals

$$\mathcal{S}_{\text{up/down}} = \left\{ \left\{ \hat{A}_{-F_k}(X_{n+1}) \pm |\hat{A}_{-F_k}(X_i) - Y_i| \right\}_{i \in F_k} \right\}_k \cup \{\pm\infty\}$$

(in standard mean regression)

- Build the predictive interval: $[q_{\alpha,\inf}(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

Theorem

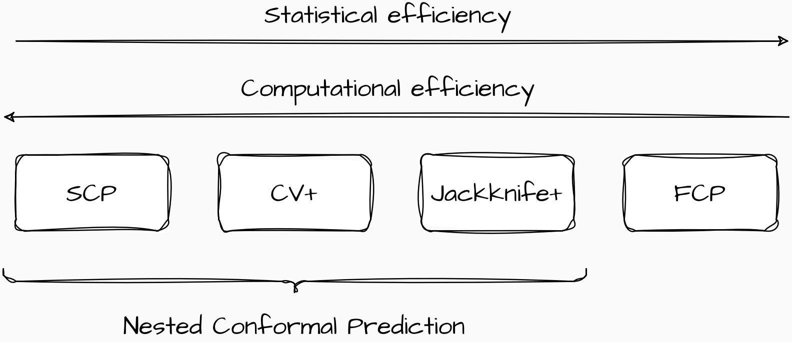
If $\mathcal{D}_n \cup (X_{n+1}, Y_{n+1})$ are exchangeable and $\mathcal{A}$ is symmetric:

$$\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})) \geq 1 - 2\alpha - \min\left(\frac{2(1-1/K)}{n/K+1}, \frac{1-K/n}{K+1}\right) \geq 1 - 2\alpha - \sqrt{2/n}.$$

[11] Barber et al. (2021b), *Predictive Inference with the jackknife+*, The Annals of Statistics

Recall $q_{\beta,\inf}(X_1, \dots, X_n) := \lfloor \beta \times n \rfloor$ smallest value of $(X_1, \dots, X_n)$

General overview



- Generalized framework encapsulating out-of-sample methods: Nested CP (Gupta et al., 2022)
- Accelerating FCP: Nouretdinov et al. (2001); Lei (2019); Ndiaye and Takeuchi (2019); Cherubin et al. (2021); Ndiaye and Takeuchi (2022); Ndiaye (2022)

Non exhaustive references.

Exchangeability does not hold in many practical applications

- CP requires exchangeable data points to ensure validity

✗ Covariate shift, i.e. $\mathcal{L}_X$ changes but $\mathcal{L}_{Y|X}$ stays constant

✗ Label shift, i.e. $\mathcal{L}_Y$ changes but $\mathcal{L}_{X|Y}$ stays constant

✗ Arbitrary distribution shift

✗ Possibly many shifts, not only one

Covariate shift (Tibshirani et al., 2019)[12]

- Setting:
  - $(X_1, Y_1), \ldots, (X_n, Y_n) \overset{i.i.d.}{\sim} P_X \times P_{Y|X}$
  - $(X_{n+1}, Y_{n+1}) \sim \tilde{P}_X \times P_{Y|X}$
- Idea: give more importance to calibration points that are closer in distribution to the test point
- In practice:
  1. estimate the likelihood ratio $w(X_i) = \dfrac{\mathrm{d}\tilde{P}_X(X_i)}{\mathrm{d}P_X(X_i)}$
  2. normalize the weights, i.e. $\omega_i = \omega(X_i) = \dfrac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)}$
  3. outputs $\widehat{C}_\alpha(X_{n+1}) =$

$$\left\{ y : \mathrm{s}\left(\hat{A}(X_{n+1}), y\right) \le q_{1-\alpha}\left(\{\omega_i S_i\}_{i \in \mathrm{Cal}} \cup \{+\infty\}\right) \right\}$$

[12] Tibshirani et al. (2019), *Conformal Prediction Under Covariate Shift*, NeurIPS

Label shift (Podkopaev and Ramdas, 2021)[13]

- Setting:
  - $(X_1, Y_1), \dots, (X_n, Y_n) \overset{i.i.d.}{\sim} P_{X|Y} \times P_Y$
  - $(X_{n+1}, Y_{n+1}) \sim P_{X|Y} \times \tilde{P}_Y$
  - Classification
- Idea: give more importance to calibration points that are closer in distribution to the test point
- Trouble: the actual test labels are unknown
- In practice:
  1. estimate the likelihood ratio $w(Y_i) = \frac{\mathrm{d}\tilde{P}_Y(Y_i)}{\mathrm{d}P_Y(Y_i)}$ using algorithms from the existing label shift literature
  2. normalize the weights, i.e. $\omega_i^y = \omega^y(X_i) = \frac{w(Y_i)}{\sum_{j=1}^n w(Y_j) + w(y)}$
  3. outputs $\widehat{C}_\alpha(X_{n+1}) =$

$$\left\{ y : \mathrm{s}\left(\hat{A}(X_{n+1}), y\right) \leq q_{1-\alpha}\left(\{\omega_i^y S_i\}_{i \in \mathrm{Cal}} \cup \{+\infty\}\right) \right\}$$

[13] Podkopaev and Ramdas (2021), *Distribution-free uncertainty quantification for classification under label shift*, UAI

Generalizations

- Arbitrary distribution shift: Cauchois et al. (2020) leverages ideas from the distributionally robust optimization literature
- Two major general theoretical results beyond exchangeability:
  - Chernozhukov et al. (2018)
    $\hookrightarrow$ If the learnt model is accurate and the data noise is strongly mixing, then CP is valid asymptotically ✓
  - Barber et al. (2022)
    $\hookrightarrow$ Quantifies the coverage loss depending on the strength of exchangeability violation
    $$\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})) \geq 1 - \alpha - \substack{\text{average violation of exchangeability} \\ \text{by each calibration point}}$$
    $\hookrightarrow$ proposed algorithm: reweighting again!
    e.g., in a temporal setting, give higher weights to more recent points.

Online setting

- Data: T_0 random variables $(X_1, Y_1), \ldots, (X_{T_0}, Y_{T_0})$ in $\mathbb{R}^d \times \mathbb{R}$
- Aim: predict the response values as well as predictive intervals for T_1 subsequent observations $X_{T_0+1}, \ldots, X_{T_0+T_1}$ sequentially: at any prediction step $t \in [\![T_0 + 1, T_0 + T_1]\!]$, $Y_{t-T_0}, \ldots, Y_{t-1}$ have been revealed
- Build the smallest interval $\widehat{C}_\alpha^t$ such that:

$$\mathbb{P}\left\{ Y_t \in \widehat{C}_\alpha^t(X_t) \right\} \geq 1 - \alpha, \quad \text{for } t \in [\![T_0 + 1, T_0 + T_1]\!],$$

often simplified in:

$$\frac{1}{T_1} \sum_{t=T_0+1}^{T_0+T_1} \mathbb{1}\left\{ Y_t \in \widehat{C}_\alpha^t(X_t) \right\} \approx 1 - \alpha.$$

Focus on the online setting

Issued from a work with:

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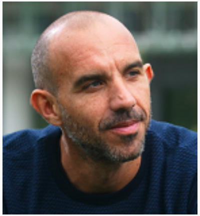

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(Online) Time series are not exchangeable

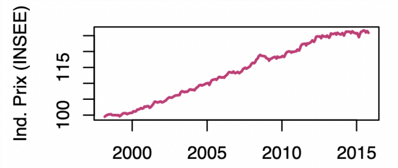


Figure 1: Trend[14]

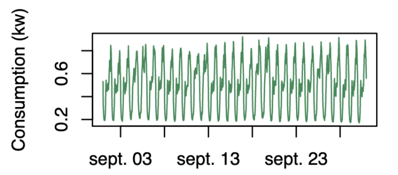


Figure 2: Seasonality[14]

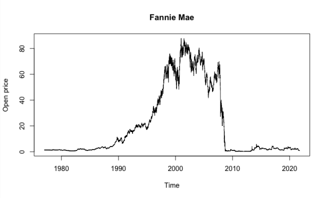


Figure 3: Shift

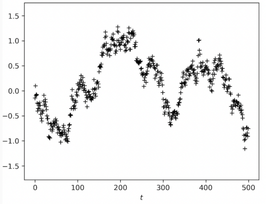


Figure 4: Time dependence

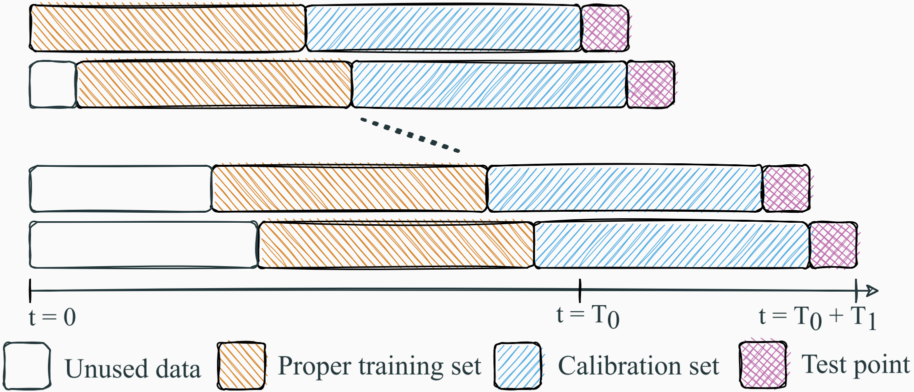
[14] Images from Yannig Goude class material.

How to adapt to time series?

Usual ideas from the time series literature:

- Consider an online procedure (for each new data, re-train and re-calibrate)
  - $\hookrightarrow$ update to recent observations (trend impact, period of the seasonality, dependence...)
- Use a sequential split
  - $\hookrightarrow$ use only the past so as to correctly estimate the variance of the residuals (using the future leads to optimistic residuals and underestimation of their variance)

Online sequential split conformal prediction (OSSCP)



Wisniewski et al. (2020); Kath and Ziel (2021); Zaffran et al. (2022)

$\hookrightarrow$ tested on real time series

Adaptive Conformal Inference (ACI), Gibbs and Candès (2021)

Refitting the model may be insufficient $\Rightarrow$ adapt the quantile level used on the calibration's scores. **(distribution shift)**

The proposed update scheme is the following:

$$\alpha_{t+1} := \alpha_t + \gamma \left(\alpha - \mathbb{1}\{ Y_t \notin \widehat{\mathcal{C}}_{\alpha_t}(X_t) \} \right) \tag{2}$$

with $\alpha_1 = \alpha$, $\gamma \geq 0$.

Intuition: if we did make an error, the interval was too small so we want to increase its length by taking a higher quantile (a smaller α_t). Reversely if we included the point.

Visualisation of the procedure

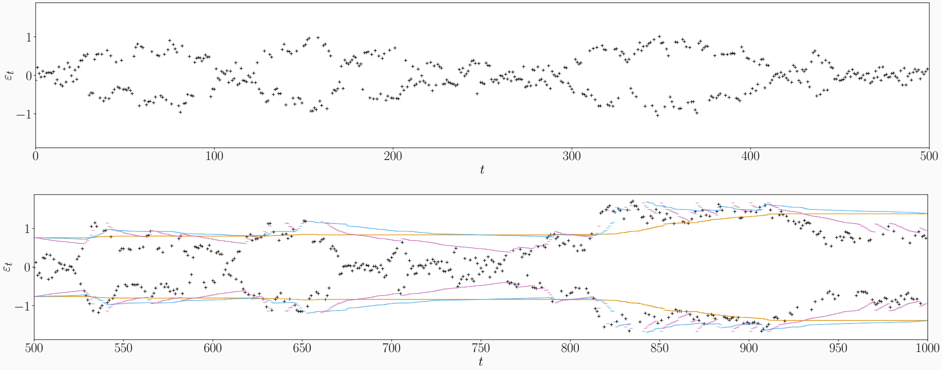


Figure 5: Visualisation of ACI with different values of γ ($\gamma = 0$, $\gamma = 0.01$, $\gamma = 0.05$)

ACI asymptotic result

Gibbs and Candès (2021) provide an asymptotic validity result for any sequence of observations.

$$\left| \frac{1}{T_1} \sum_{t=T_0+1}^{T_0+T_1} \mathbb{1}\left\{ Y_t \in \widehat{\mathcal{C}}_{\alpha_t}\left(X_t\right) \right\} - (1-\alpha) \right| \leq \frac{2}{\gamma T_1}$$

$\Rightarrow$ favors large γ. But, the higher γ, the more frequent are the infinite intervals.

Approach

Aim: derive theoretical results on the **average length** of ACI depending on γ

$\hookrightarrow$ Guideline for choosing γ

Approach:

- consider extreme cases (useful in an online context) with simple theoretical distributions
  1. exchangeable
  2. Auto-Regressive case (AR(1))
- Assume the calibration is perfect (and more), to rely on Markov Chain theory

Define $L(\alpha_t) = 2Q(1-\alpha_t)$ the length of the interval predicted by the adaptive algorithm at time t, and $L_0 = 2Q(1-\alpha)$ the length of the interval predicted by the non-adaptive algorithm ($\gamma = 0$).

Theorem

Assume the scores are exchangeable with quantile function Q perfectly estimated at each time, and other assumptions.

Then, for all $\gamma > 0$, $(\alpha_t)_{t>0}$ forms a Markov Chain, that admits a stationary distribution π_γ, and

$$\frac{1}{T}\sum_{t=1}^{T} L(\alpha_t) \xrightarrow[T\to+\infty]{a.s.} \mathbb{E}_{\pi_\gamma}[L] \overset{not.}{=} \mathbb{E}_{\tilde{\alpha}\sim\pi_\gamma}[L(\tilde{\alpha})].$$

Moreover, as $\gamma \to 0$,

$$\mathbb{E}_{\pi_\gamma}[L] = L_0 + Q''(1-\alpha)\frac{\gamma}{2}\alpha(1-\alpha) + O(\gamma^{3/2}).$$

Numerical analysis of ACI's length: AR(1) case

Theorem

Assume the residuals follow an AR(1) process: $\hat{\varepsilon}_{t+1} = \varphi \hat{\varepsilon}_t + \xi_{t+1}$ with $(\xi_t)_t$ i.i.d. random variables and other assumptions, we have:

$$\frac{1}{T} \sum_{t=1}^{T} L(\alpha_t) \underset{T \to +\infty}{\overset{a.s.}{\longrightarrow}} \mathbb{E}_{\pi_{\gamma,\varphi}}[L].$$

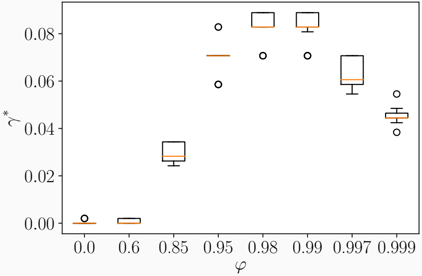


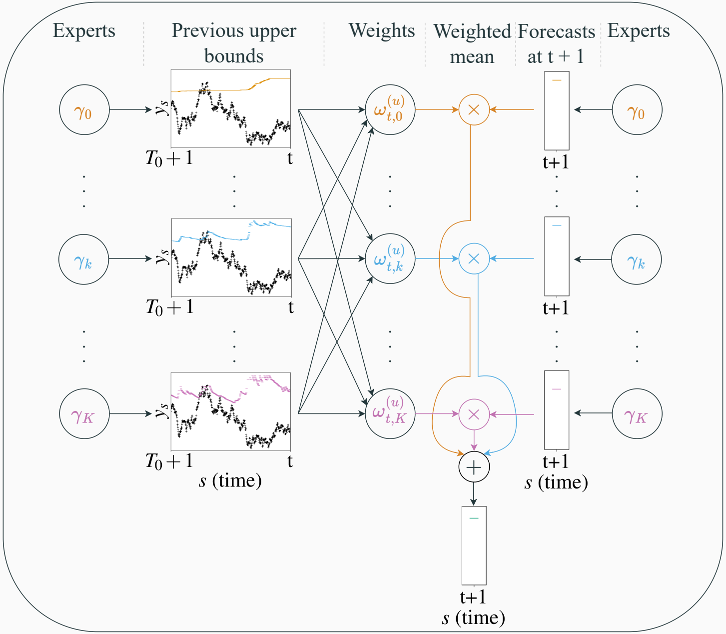
Figure 6: γ^* minimizing the average length for each φ.

AgACI: adaptive wrapper around ACI

Online aggregation under expert advice (Cesa-Bianchi and Lugosi, 2006) computes an optimal weighted mean of experts.

`AgACI` performs 2 independent aggregations: one for each bound (the upper and lower ones).

AgACI: adaptive wrapper around ACI, scheme (upper bound)



Data generation and simulation settings

$$Y_t = 10\sin(\pi X_{t,1}X_{t,2}) + 20(X_{t,3} - 0.5)^2 + 10X_{t,4} + 5X_{t,5} + \varepsilon_t$$

where the $X_{t,\cdot} \sim \mathcal{U}([0,1])$ and ε_t is an ARMA(1,1) process:

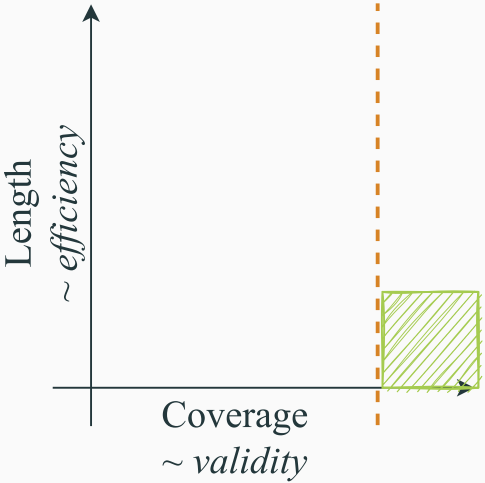
$$\varepsilon_{t+1} = \varphi\varepsilon_t + \xi_{t+1} + \theta\xi_t,$$

with ξ_t is a white noise of variance σ^2.

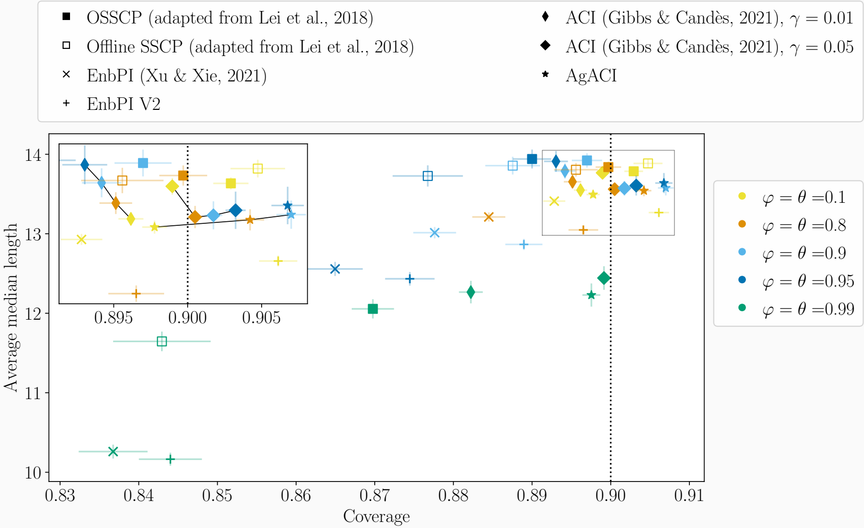
- $\varphi = \theta$ range in $[0.1, 0.8, 0.9, 0.95, 0.99]$.
- We fix σ to keep the variance $\mathrm{Var}(\varepsilon_t)$ constant to 10 (or 1).
- We use random forest as regressor.
- For each setting (pair variance and φ,θ):
    - 300 points, the last 100 kept for prediction and evaluation,
    - 500 repetitions,

  $\Rightarrow$ in total, $100 \times 500 = 50000$ predictions are evaluated.

Visualisation of the results



Results: impact of the temporal dependence, ARMA(1,1), variance 10



Summary

1. The temporal dependence impacts the *validity*.
2. Online is significantly better than offline.
3. **OSSCP.** Achieves *valid* coverage for φ and θ smaller than 0.9, but is not robust to the increasing dependence.
4. **EnbPI.** Its *validity* strongly depends on the data distribution. When the method is *valid*, it produces the smallest intervals. EnbPI V2 method should be preferred.
5. **ACI.** Achieves *valid* coverage for every simulation settings with a well chosen γ, or for dependence such that $\varphi < 0.95$. It is robust to the strength of the dependence.
6. **AgACI.** Achieves *valid* coverage for every simulation settings, with good *efficiency*.

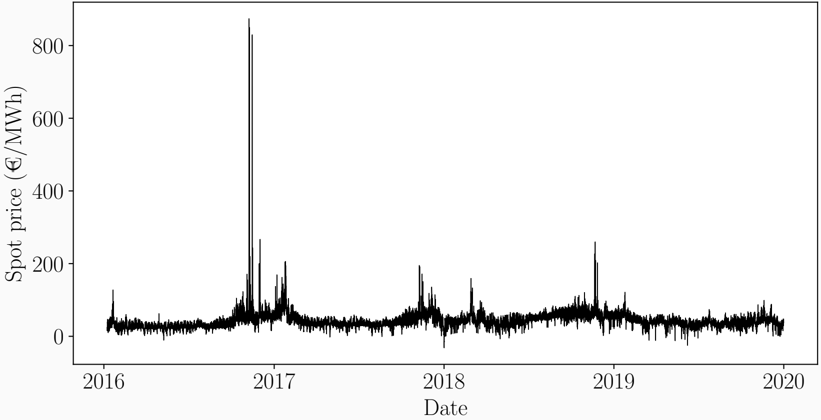


Figure 7: Representation of the French electricity spot price, from 2016 to 2019.

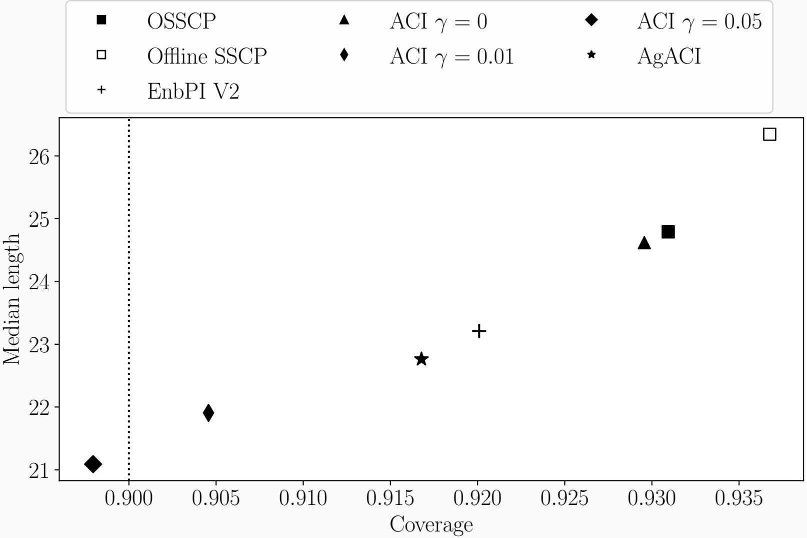
Forecasting electricity prices with confidence in 2019

- Forecast for the year 2019.
- Random forest regressor.
- One model per hour, we concatenate the predictions afterwards.

$\hookrightarrow$ 24 models

  - $y_t \in \mathbb{R}$
  - $x_t \in \mathbb{R}^d$, with $d = 24 + 24 + 1 + 7 = 56$
  - 3 years for training/calibration, i.e. $T_0 = 1096$ observations
  - 1 year to forecast, i.e. $T_1 = 365$ observations

Performance on predicted French electricity Spot price for the year 2019



Performance on predicted French electricity Spot price: visualisation of a day

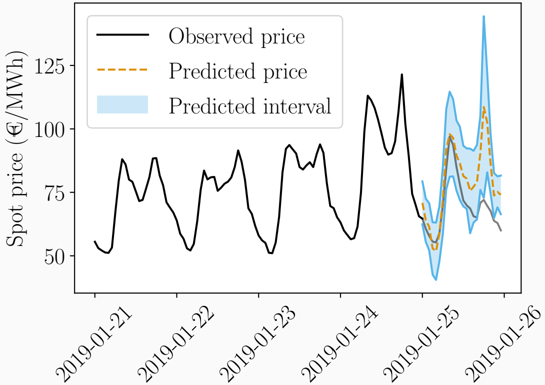


Figure 8: French electricity spot price, its prediction and its uncertainty with AgACI.

Take-home-messages on this subsection

- Theoretical results on ACI's length depending on γ
- ACI useful for time series with general dependency (extensive synthetic experiments and real data)
- Empirical proposition of an adaptive choice of γ: `AgACI`

Recent developments

- Gibbs and Candès (2022) later on also proposes a method not requiring to choose γ
- Bhatnagar et al. (2023) enjoys **anytime** regret bound, by leveraging tools from the strongly adaptive regret minimization literature
- Bastani et al. (2022) proposes an algorithm achieving stronger coverage guarantees (conditional on specified overlapping subsets, and threshold calibrated) without hold-out set
- Angelopoulos et al. (2023) combines CP ideas with control theory ones, to adaptively improve the predictive intervals depending on the errors structure

Non exhaustive references.

Useful resources on Conformal Prediction (non exhaustive)

- Book reference: Vovk et al. (2005) *(new edition in 2022)*
- A gentle tutorial:
  - Angelopoulos and Bates (2023)
  - `Videos playlist`
- Another tutorial: Fontana et al. (2023)
- `GitHub repository` with plenty of links: Manokhin (2022)

Angelopoulos, A. N. and Bates, S. (2023). Conformal prediction: A gentle introduction. *Foundations and Trends® in Machine Learning*, 16(4).

Angelopoulos, A. N., Candès, E. J., and Tibshirani, R. J. (2023). Conformal pid control for time series prediction. arXiv: 2307.16895.

Barber, R. F., Candès, E. J., Ramdas, A., and Tibshirani, R. J. (2021a). The limits of distribution-free conditional predictive inference. *Information and Inference: A Journal of the IMA*, 10(2).

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

Barber, R. F., Candès, E. J., Ramdas, A., and Tibshirani, R. J. (2022). Conformal prediction beyond exchangeability. To appear in *Annals of Statistics (2023)*.

Bastani, O., Gupta, V., Jung, C., Noarov, G., Ramalingam, R., and Roth, A. (2022). Practical adversarial multivalid conformal prediction. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Bhatnagar, A., Wang, H., Xiong, C., and Bai, Y. (2023). Improved online conformal prediction via strongly adaptive online learning. In *Proceedings of the 40th International Conference on Machine Learning*. PMLR.

Cauchois, M., Gupta, S., Ali, A., and Duchi, J. C. (2020). Robust Validation: Confident Predictions Even When Distributions Shift. arXiv: 2008.04267.

Cesa-Bianchi, N. and Lugosi, G. (2006). *Prediction, learning, and games*. Cambridge University Press.

Chernozhukov, V., Wüthrich, K., and Yinchu, Z. (2018). Exact and Robust Conformal Inference Methods for Predictive Machine Learning with Dependent Data. In *Conference On Learning Theory*. PMLR.

Chernozhukov, V., Wüthrich, K., and Zhu, Y. (2021). Distributional conformal prediction. *Proceedings of the National Academy of Sciences*, 118(48).

Cherubin, G., Chatzikokolakis, K., and Jaggi, M. (2021). Exact optimization of conformal predictors via incremental and decremental learning. In *Proceedings of the 38th International Conference on Machine Learning*. PMLR.

Fontana, M., Zeni, G., and Vantini, S. (2023). Conformal prediction: A unified review of theory and new challenges. *Bernoulli*, 29(1).

Gibbs, I. and Candès, E. (2021). Adaptive conformal inference under distribution shift. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Gibbs, I. and Candès, E. (2022). Conformal inference for online prediction with arbitrary distribution shifts. arXiv: 2208.08401.

Gibbs, I., Cherian, J. J., and Candès, E. J. (2023). Conformal prediction with conditional guarantees. arXiv: 2305.12616.

Guan, L. (2022). Localized conformal prediction: a generalized inference framework for conformal prediction. *Biometrika*, 110(1).

Gupta, C., Kuchibhotla, A. K., and Ramdas, A. (2022). Nested conformal prediction and quantile out-of-bag ensemble methods. *Pattern Recognition*, 127.

Izbicki, R., Shimizu, G., and Stern, R. B. (2022). CD-split and HPD-split: Efficient conformal regions in high dimensions. *Journal of Machine Learning Research*, 23(87).

Jung, C., Noarov, G., Ramalingam, R., and Roth, A. (2023). Batch multivalid conformal prediction. In *International Conference on Learning Representations*.

Kath, C. and Ziel, F. (2021). Conformal prediction interval estimation and applications to day-ahead and intraday power markets. *International Journal of Forecasting*, 37(2).

Kivaranovic, D., Johnson, K. D., and Leeb, H. (2020). Adaptive, Distribution-Free Prediction Intervals for Deep Networks. In *International Conference on Artificial Intelligence and Statistics*. PMLR.

Lei, J. (2019). Fast exact conformalization of the lasso using piecewise linear homotopy. *Biometrika*, 106(4).

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*.

Lei, J. and Wasserman, L. (2014). Distribution-free prediction bands for non-parametric regression. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 76(1).

Manokhin, V. (2022). Awesome conformal prediction. https://github.com/valeman/awesome-conformal-prediction.

Ndiaye, E. (2022). Stable conformal prediction sets. In *Proceedings of the 39th International Conference on Machine Learning*. PMLR.

Ndiaye, E. and Takeuchi, I. (2019). Computing full conformal prediction set with approximate homotopy. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Ndiaye, E. and Takeuchi, I. (2022). Root-finding approaches for computing conformal prediction set. *Machine Learning*, 112(1).

Nouretdinov, I., Melluish, T., and Vovk, V. (2001). Ridge regression confidence machine. In *Proceedings of the 18th International Conference on Machine Learning*.

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

Podkopaev, A. and Ramdas, A. (2021). Distribution-free uncertainty quantification for classification under label shift. In *Proceedings of the Thirty-Seventh Conference on Uncertainty in Artificial Intelligence*. PMLR.

Romano, Y., Barber, R. F., Sabatti, C., and Candès, E. (2020a). With Malice Toward None: Assessing Uncertainty via Equalized Coverage. *Harvard Data Science Review*, 2(2).

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

Romano, Y., Sesia, M., and Candes, E. (2020b). Classification with valid and adaptive coverage. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Sesia, M. and Romano, Y. (2021). Conformal prediction using conditional histograms. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Tibshirani, R. J., Barber, R. F., Candes, E., and Ramdas, A. (2019). Conformal Prediction Under Covariate Shift. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc.

Vovk, V. (2012). Conditional Validity of Inductive Conformal Predictors. In *Asian Conference on Machine Learning*. PMLR.

Vovk, V. (2015). Cross-conformal predictors. *Annals of Mathematics and Artificial Intelligence*, 74(1-2).

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

Wisniewski, W., Lindsay, D., and Lindsay, S. (2020). Application of conformal prediction interval estimations to market makers' net positions. In *Proceedings of the Ninth Symposium on Conformal and Probabilistic Prediction and Applications*, volume 128. PMLR.

Zaffran, M., Féron, O., Goude, Y., Josse, J., and Dieuleveut, A. (2022). Adaptive conformal predictions for time series. In *Proceedings of the 39th International Conference on Machine Learning*. PMLR.