

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

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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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- 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

- **Data:** $(X_i, Y_i)_{i=1}^n \in (\mathbb{R}^d, \mathcal{Y})^n$

- **Goal:** Learn a function \hat{f} such that

$$\underbrace{i \in \llbracket 1, n \rrbracket : \hat{f}(X_i) \simeq Y_i}_{\text{training data}} \quad \text{and moreover}$$

$$\underbrace{\hat{f}(X_{n+1}) \simeq Y_{n+1}}_{\text{prediction on test (unseen) data}}$$

- 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

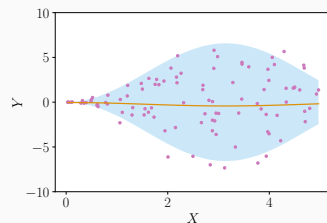
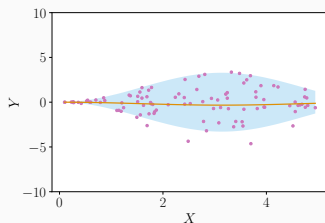
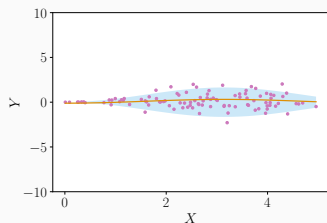
- **Loss function:** $\ell(Y, f(X))$ evaluates how close $f(X)$ is to Y
 - Classification \rightsquigarrow 0-1 loss: $\ell(Y, f(X)) = \mathbb{1}_{Y \neq f(X)}$
 - Regression \rightsquigarrow Quadratic loss: $\ell(Y, f(X)) = (Y - f(X))^2$
- \hat{f} should be as good as possible over all the possible X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

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

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

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

On the importance of quantifying uncertainty



↪ Same **predictions**, yet 3 distinct underlying phenomena!

⇒ **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)

Median regression

- The Bayes predictor depends on the chosen **loss function**.

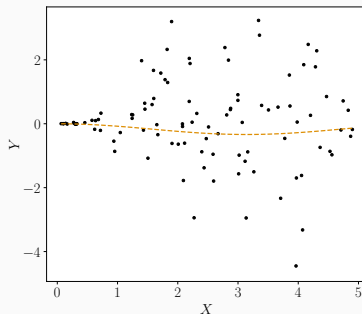
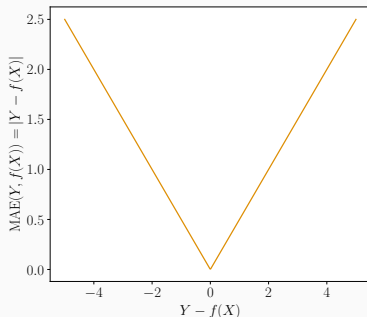
↪ **Bayes predictor** $f^* \in \operatorname{argmin}_f \operatorname{Risk}_\ell(f)$

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

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

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

$$\Rightarrow f^*(X) = \operatorname{median} [Y|X] = Q_{Y|X}(0.5)$$



Generalization: Quantile regression

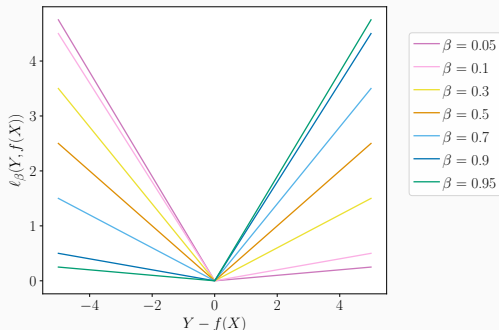
- Quantile level $\beta \in [0, 1]$
- Pinball loss

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

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

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

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



- Link between the **pinball loss** and the **quantiles**?

Set $q^* \in \arg \min_q \mathbb{E}[\ell_\beta(Y - q)]$. Then,

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

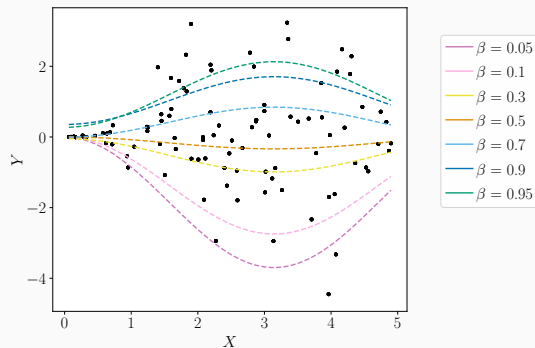
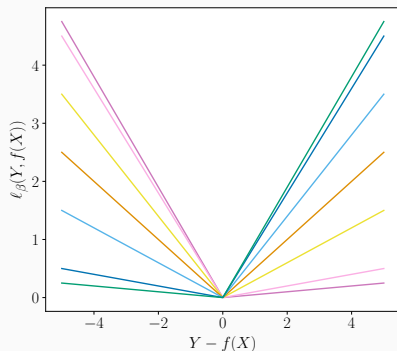
$$0 = (\beta - 1)F_Y(q^*) + \beta(1 - F_Y(q^*))$$

$$(1 - \beta)F_Y(q^*) = \beta(1 - F_Y(q^*))$$

$$\beta = F_Y(q^*)$$

$$\Leftrightarrow q^* = F_Y^{-1}(\beta)$$

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}_α such that:

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

and \mathcal{C}_α 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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Standard regression case

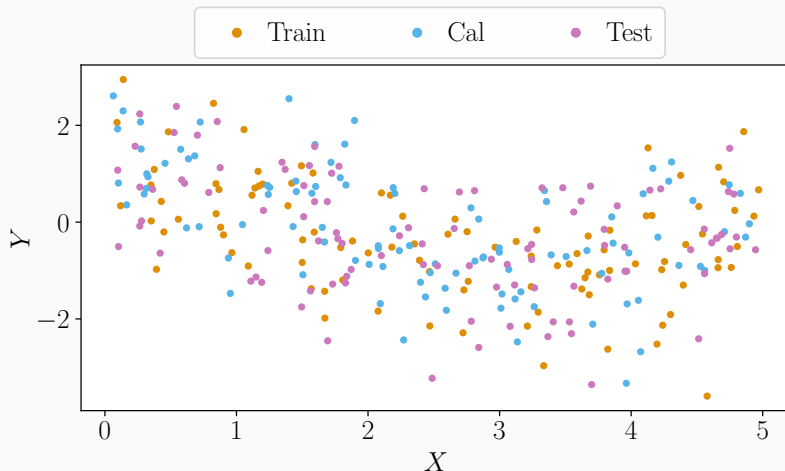
Conformalized Quantile Regression (CQR)

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Split Conformal Prediction (SCP)^{1,2,3}: toy example

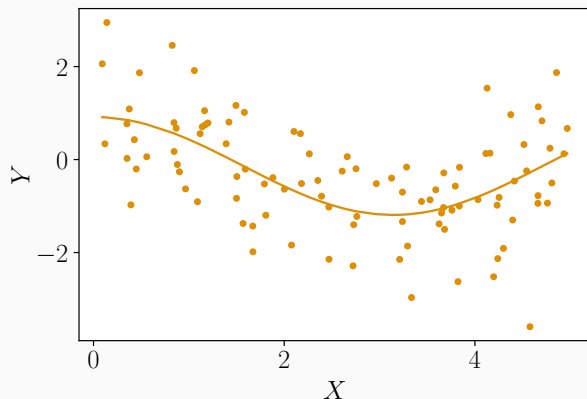


¹Vovk et al. (2005), *Algorithmic Learning in a Random World*

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

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

Split Conformal Prediction (SCP)^{1,2,3}: training step



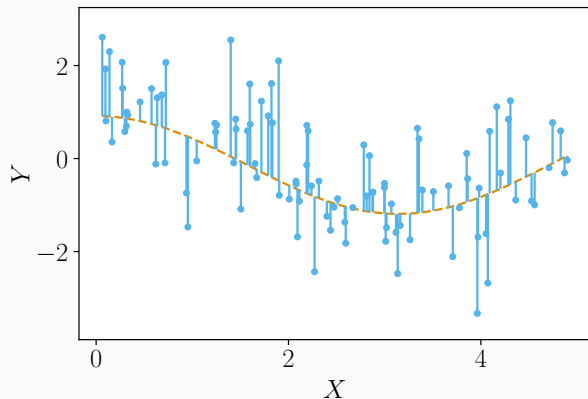
► Learn (or get) $\hat{\mu}$

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Split Conformal Prediction (SCP)^{1,2,3}: calibration step



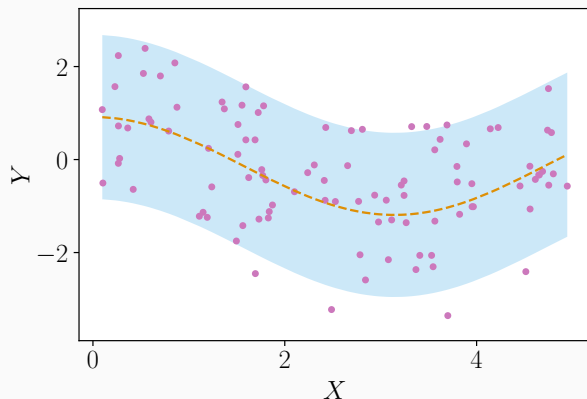
- Predict with $\hat{\mu}$
- Get the `|residuals|`, a.k.a. conformity scores
- Compute the $(1 - \alpha)$ empirical quantile of $\mathcal{S} = \{|residuals|\}_{\text{Cal}} \cup \{+\infty\}$, noted $q_{1-\alpha}(\mathcal{S})$

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Split Conformal Prediction (SCP)^{1,2,3}: prediction step



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

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SCP: implementation details



1. Randomly split the training data into a **proper training set** (size $\#Tr$) and a **calibration set** (size $\#Cal$)
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 $\#Cal + 1$ **conformity scores**:

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

(+ 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

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

SCP: implementation details



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

5. Compute the $(1 - \alpha) \left(\frac{1}{\#Cal} + 1 \right)$ quantile of these scores, noted $q_{1-\alpha}(\mathcal{S})$
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$$\hat{C}_\alpha(X_{n+1}) = [\hat{\mu}(X_{n+1}) - q_{1-\alpha}(\mathcal{S}); \hat{\mu}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$$

Definition (Exchangeability)

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

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

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 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 $\hat{C}_\alpha(\cdot)$ such that:

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

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

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

⁴Only 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 $\beta \in]0, 1[$:

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

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

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

When $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable, the scores $\{S_i\}_{i \in \text{Cal}} \cup \{S_{n+1}\}$ 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 :

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

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

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

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

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

□

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

Theorem

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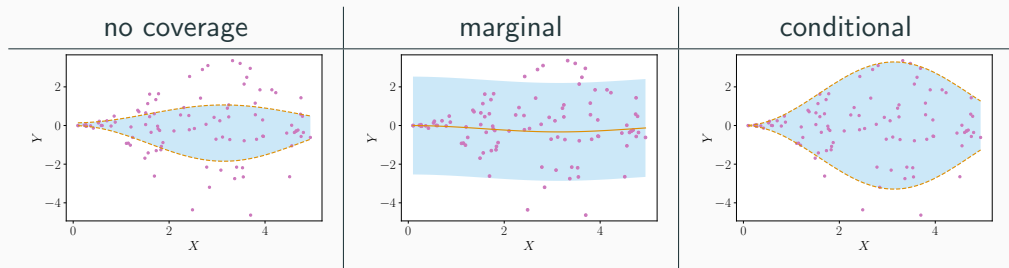
$$\mathbb{P} \left\{ Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \right\} \leq 1 - \alpha + \frac{1}{\#\text{Cal} + 1}.$$

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

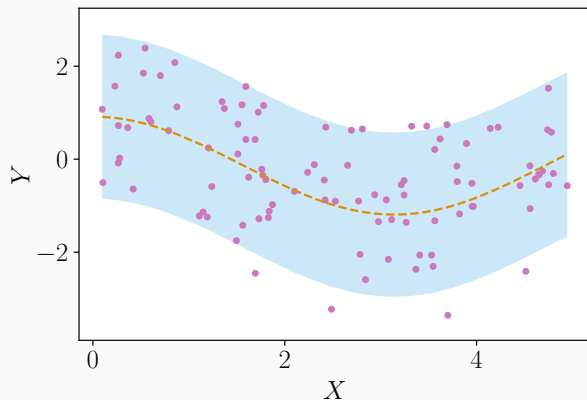
⁴Only the calibration and test data need to be exchangeable.

Conditional coverage implies adaptiveness

- **Marginal** coverage: $\mathbb{P} \left\{ Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \right\}$ the errors may differ across regions of the input space (i.e. non-adaptive)
- **Conditional** coverage: $\mathbb{P} \left\{ Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) | X_{n+1} \right\}$ 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 $\hat{C}_\alpha(x)$: $[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$

Informative conditional coverage as such is impossible

- Impossibility results

↪ Lei and Wasserman (2014); Vovk (2012); Barber et al. (2021a)

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

- Approximate conditional coverage

↪ Romano et al. (2020a); Guan (2022); Jung et al. (2023); Gibbs et al. (2023)

Target $\mathbb{P}(Y_{n+1} \in \hat{C}_\alpha | X_{n+1} \in \mathcal{R}(x)) \geq 1 - \alpha$

- Asymptotic (with the sample size) conditional coverage

↪ Romano et al. (2019); Kivaranovic et al. (2020); Chernozhukov et al. (2021); Sesia and Romano (2021); Izbicki et al. (2022)

Supervised learning context and quantile regression

Split Conformal Prediction (SCP)

Standard regression case

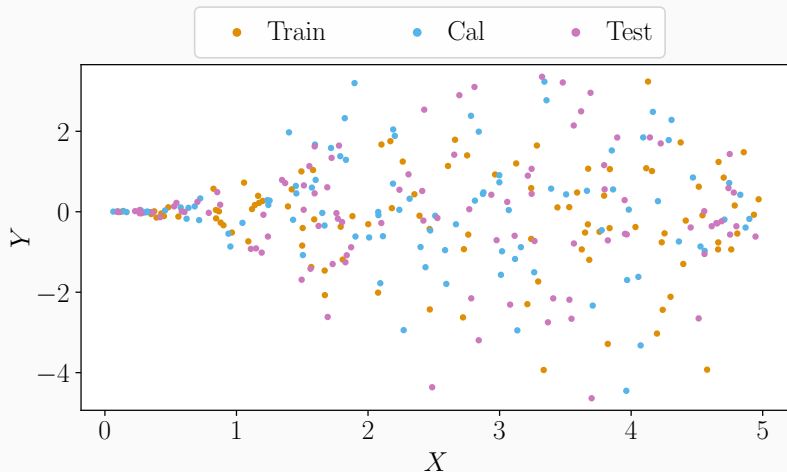
Conformalized Quantile Regression (CQR)

Generalization of SCP: going beyond regression

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

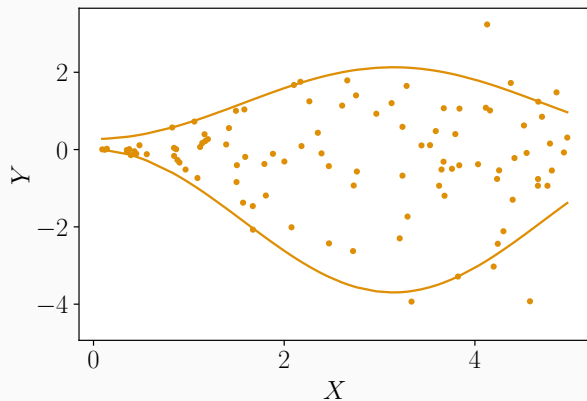
Beyond exchangeability

Conformalized Quantile Regression (CQR)⁵



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

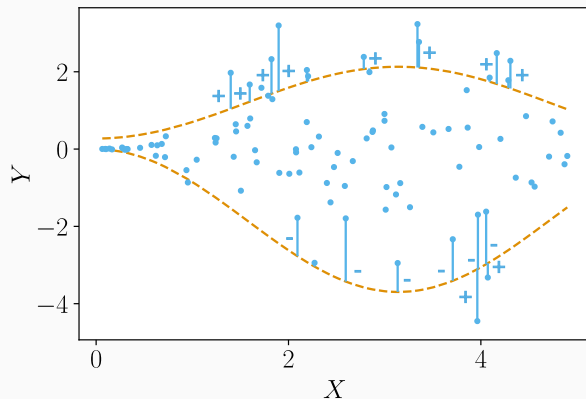
Conformalized Quantile Regression (CQR)⁵: training step



► Learn (or get) $\widehat{QR}_{\text{lower}}$ and $\widehat{QR}_{\text{upper}}$

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

Conformalized Quantile Regression (CQR)⁵: calibration step

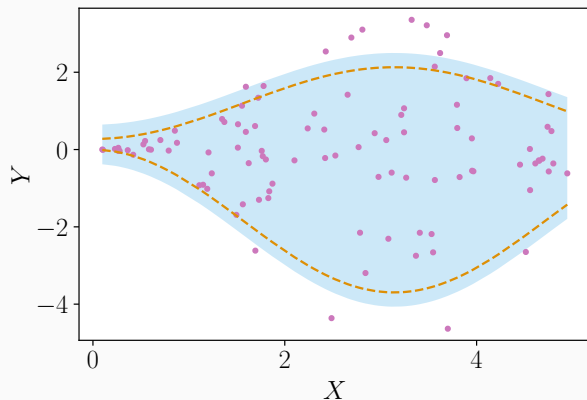


- ▶ Predict with \widehat{QR}_{lower} and \widehat{QR}_{upper}
- ▶ Get the scores
 $\mathcal{S} = \{S_i\}_{\text{Cal}} \cup \{+\infty\}$
- ▶ Compute the $(1 - \alpha)$ empirical quantile of \mathcal{S} , noted $q_{1-\alpha}(\mathcal{S})$

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

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

Conformalized Quantile Regression (CQR)⁵: prediction step



► Predict with \widehat{QR}_{lower} and \widehat{QR}_{upper}

► Build

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

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

CQR: implementation details



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

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

CQR: implementation details

1. Randomly split the training data into a **proper training set** (size $\#Tr$) and a **calibration set** (size $\#Cal$)
2. Get \widehat{QR}_{lower} and \widehat{QR}_{upper} by training the algorithm \mathcal{A} on the **proper training set**

3. Obtain a set of $\#Cal$ **conformity scores** \mathcal{S} :

$$\mathcal{S} = \{S_i = \max\left(\widehat{QR}_{lower}(X_i) - Y_i, Y_i - \widehat{QR}_{upper}(X_i)\right), i \in Cal\}$$

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

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

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 $\hat{C}_\alpha(\cdot)$ such that:

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

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

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

Proof: application of the quantile lemma.

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

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

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Generalization of SCP: going beyond regression

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SCP is defined by the conformity score function



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

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

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

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

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

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

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 $\hat{C}_\alpha(\cdot)$ such that:

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

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

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

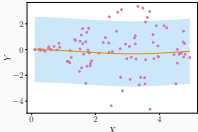
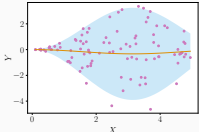
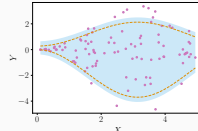
Proof: application of the quantile lemma.

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

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

SCP: what choices for the regression scores?

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

	Standard SCP Vovk et al. (2005)	Locally weighted SCP Lei et al. (2018)	CQR Romano et al. (2019)
$s(\hat{A}(X), Y)$	$ \hat{\mu}(X) - Y $	$\frac{ \hat{\mu}(X) - Y }{\hat{\rho}(X)}$	$\max(\hat{Q}R_{\text{lower}}(X) - Y, Y - \hat{Q}R_{\text{upper}}(X))$
$\hat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(S)]$	$[\hat{\mu}(x) \pm q_{1-\alpha}(S)\hat{\rho}(x)]$	$[\hat{Q}R_{\text{lower}}(x) - q_{1-\alpha}(S); \hat{Q}R_{\text{upper}}(x) + q_{1-\alpha}(S)]$
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

- $Y \in \{1, \dots, C\}$ (C classes)
- $\hat{A}(X) = (\hat{p}_1(X), \dots, \hat{p}_C(X))$ (estimated probabilities)
- $s(\hat{A}(X), Y) := 1 - (\hat{A}(X))_Y$
- For a new point X_{n+1} , return
$$\hat{C}_\alpha(X_{n+1}) = \{y \text{ such that } s(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\mathcal{S})\}$$

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

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

"dog" $\notin \hat{C}_\alpha(X_{n+1})$
"tiger" $\in \hat{C}_\alpha(X_{n+1})$
"cat" $\in \hat{C}_\alpha(X_{n+1})$

Ex: $Y \in \{\text{"dog"}, \text{"tiger"}, \text{"cat"}\}$, 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	0.05	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

- $q_{1-\alpha}(\mathcal{S}) = 0.45$

- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

$$\hookrightarrow s(\hat{A}(X_{n+1}), \text{"dog"}) = 0.95$$

$$\hookrightarrow s(\hat{A}(X_{n+1}), \text{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$$

$$\hookrightarrow s(\hat{A}(X_{n+1}), \text{"cat"}) = 0.65$$

$$\text{"dog"} \notin \hat{C}_\alpha(X_{n+1})$$

$$\text{"tiger"} \in \hat{C}_\alpha(X_{n+1})$$

$$\text{"cat"} \notin \hat{C}_\alpha(X_{n+1})$$

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

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!)

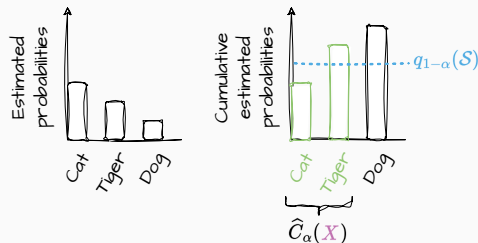
⇒ Other score functions can be built to improve adaptiveness

(as in regression with localized scores)

SCP: classification with Adaptive Prediction Sets⁸

1. Sort in decreasing order $\hat{p}_{\sigma(1)}(X) \geq \dots \geq \hat{p}_{\sigma(C)}(X)$
2. $\mathbf{s}(\hat{A}(X), Y) := \sum_{k=1}^{\sigma^{-1}(Y)} \hat{p}_{\sigma(k)}(X)$ (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 $\{\sigma_{n+1}(1), \dots, \sigma_{n+1}(r^*)\}$, where

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



⁸Romano 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: $Y \in \{\text{"dog"}, \text{"tiger"}, \text{"cat"}\}$, 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	0.05	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: $\hat{A}(X_{n+1}) = (0.05, 0.45, 0.5), r^* = 2$

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

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

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

- **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 :

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

↪ marginal also over the whole calibration set and the test point!

Challenges: open questions (non exhaustive!)

- Conditional coverage
- Computational cost vs statistical power
- Exchangeability

(~ Previous Section)

(Next Section)

(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

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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 $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$.
 - compute the empirical quantile $q_{1-\alpha}(\mathcal{S})$ of the set of scores

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

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

✗ \hat{A} has been obtained using the training set $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ but did not use X_{n+1} .

$\Rightarrow \mathbf{s} \left(\hat{A}(X_{n+1}), y \right)$ stochastically dominates any element of $\left\{ \mathbf{s} \left(\hat{A}(X_i), Y_i \right) \right\}_{i=1}^n$.

Full Conformal Prediction⁹ 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.

⁹Vovk 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 $\{(X_1, Y_1), \dots, (X_n, Y_n)\} \cup \{(X_{n+1}, y)\}$

2. Obtain a set of training scores

$$\mathcal{S}^{(\text{train})} = \left\{ s(\hat{A}_y(X_i), Y_i) \right\}_{i=1}^n \cup \{ s(\hat{A}_y(X_{n+1}), y) \}$$

and compute their $1 - \alpha$ empirical quantile $q_{1-\alpha}(\mathcal{S}^{(\text{train})})$

3. Output the set $\{ y \text{ such that } s(\hat{A}_y(X_{n+1}), y) \leq q_{1-\alpha}(\mathcal{S}^{(\text{train})}) \}$

✓ Test point treated in the same way than train points

✗ Computationally costly

Definition (Symmetrical algorithm)

A deterministic algorithm $\mathcal{A} : (U_1, \dots, U_n) \mapsto \hat{A}$ is **symmetric** if for any permutation σ of $\llbracket 1, n \rrbracket$:

$$\mathcal{A}(U_1, \dots, U_n) \stackrel{\text{a.s.}}{=} \mathcal{A}(U_{\sigma(1)}, \dots, U_{\sigma(n)}) .$$

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 $\hat{C}_\alpha(\cdot)$ such that:

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

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

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

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

FCP sets with an interpolating algorithm

Assume \mathcal{A} interpolates:

- $\hat{A} = \mathcal{A}((x_1, y_1), \dots, (x_{n+1}, y_{n+1}))$
- $\hat{A}(x_k) - y_k = 0$ for any $k \in \llbracket 1, n+1 \rrbracket$

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

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Full Conformal Prediction

Jackknife+

Beyond exchangeability

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} .

- 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 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)

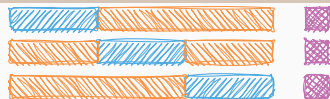
- Build the predictive interval: $[q_{\alpha, \text{inf}}(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

Theorem

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

¹⁰ Barber et al. (2021b), *Predictive Inference with the jackknife+*, The Annals of Statistics

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



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

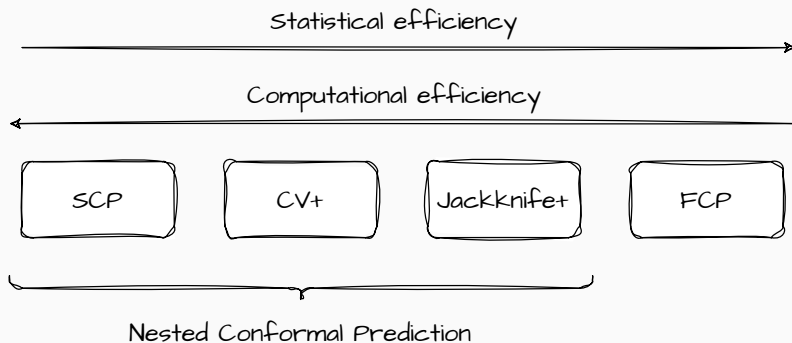
Theorem

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

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

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

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



- 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)

Supervised learning context and quantile regression

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Beyond exchangeability

- Some short literature review

- Focus on the online setting

- Theoretical analysis of ACI's length

- AgACI

- Simulated data and real industrial application

- Concluding remarks

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Concluding remarks

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

- **Setting:**
 - $(X_1, Y_1), \dots, (X_n, Y_n) \stackrel{i.i.d.}{\sim} P_X \times P_{Y|X}$
 - $(X_{n+1}, Y_{n+1}) \sim \tilde{P}_X \times P_{Y|X}$
- **Idea:** give more importance to calibration points that are closer in distribution to the test point
- **In practice:**

1. estimate the **likelihood ratio** $w(X_i) = \frac{d\tilde{P}_X(X_i)}{dP_X(X_i)}$
2. normalize the weights, i.e. $\omega_i = \omega(X_i) = \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)}$
3. outputs $\hat{C}_\alpha(X_{n+1}) = \left\{ y : \mathbf{s}(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\{\omega_i S_i\}_{i \in \text{Cal}} \cup \{+\infty\}) \right\}$

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

- **Setting:**
 - $(X_1, Y_1), \dots, (X_n, Y_n) \stackrel{i.i.d.}{\sim} P_{X|Y} \times P_Y$
 - $(X_{n+1}, Y_{n+1}) \sim P_{X|Y} \times \tilde{P}_Y$
 - **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** $w(Y_i) = \frac{d\tilde{P}_Y(Y_i)}{dP_Y(Y_i)}$ 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 $\hat{C}_\alpha(X_{n+1}) = \left\{ y : \mathbf{s}(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}(\{\omega_i^y S_i\}_{i \in \text{Cal}} \cup \{+\infty\}) \right\}$

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

- 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)
 - ↪ If the learnt model is accurate and the data noise is strongly mixing, then CP is valid asymptotically ✓
 - Barber et al. (2022)
 - ↪ Quantifies the coverage loss depending on the strength of exchangeability violation
 - $$\mathbb{P}(Y_{n+1} \in \hat{C}_\alpha(X_{n+1})) \geq 1 - \alpha - \text{average violation of exchangeability by each calibration point}$$
 - ↪ proposed algorithm: **reweighting** again!
 - e.g., in a temporal setting, give higher weights to more recent points.

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

$$\mathbb{P} \left\{ Y_t \in \hat{C}_\alpha^t(X_t) \right\} \geq 1 - \alpha, \text{ for } t \in \llbracket T_0 + 1, T_0 + T_1 \rrbracket,$$

often simplified in:

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

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(Online) Time series are not exchangeable

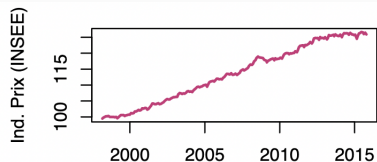


Figure 1: Trend¹⁴

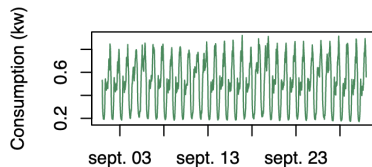


Figure 2: Seasonality¹⁴

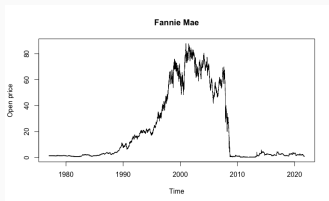


Figure 3: Shift

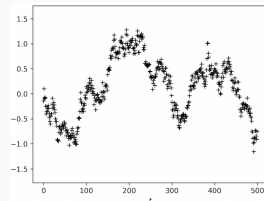


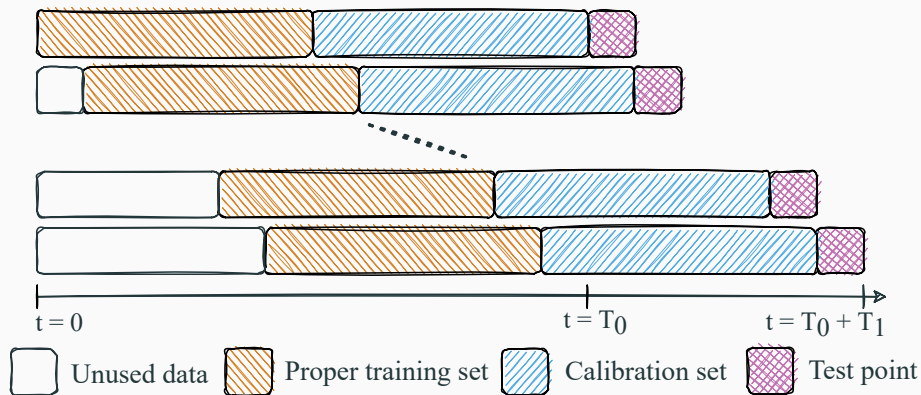
Figure 4: Time dependence

¹⁴Images from Yannig Goude class material.

Usual ideas from the time series literature:

- Consider an online procedure (for each new data, re-train and re-calibrate)
 - ↪ update to recent observations (trend impact, period of the seasonality, dependence...)
- Use a sequential split
 - ↪ 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)

↪ tested on real time series

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:

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

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

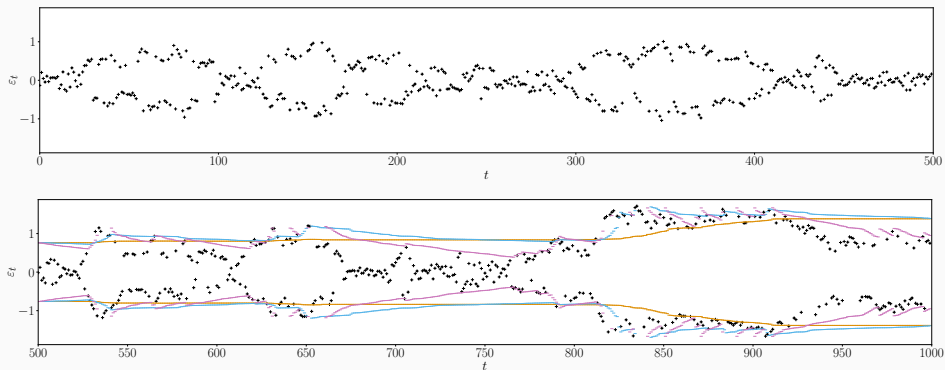


Figure 5: Visualisation of ACI with different values of γ ($\gamma = 0$, $\gamma = 0.01$, $\gamma = 0.05$)

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

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

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

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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

Theoretical analysis of ACI's length: exchangeable case

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

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

Moreover, as $\gamma \rightarrow 0$,

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

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:

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

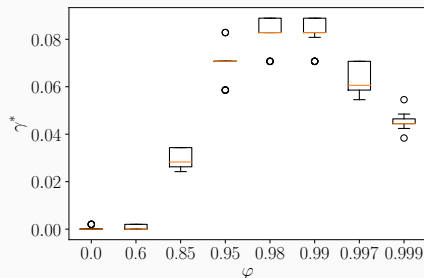


Figure 6: γ^* minimizing the average length for each φ .

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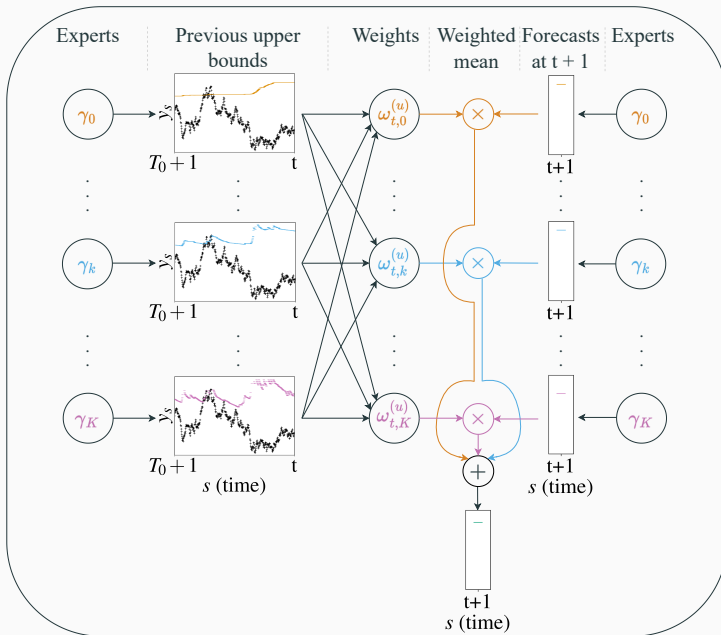
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Concluding remarks

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)



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

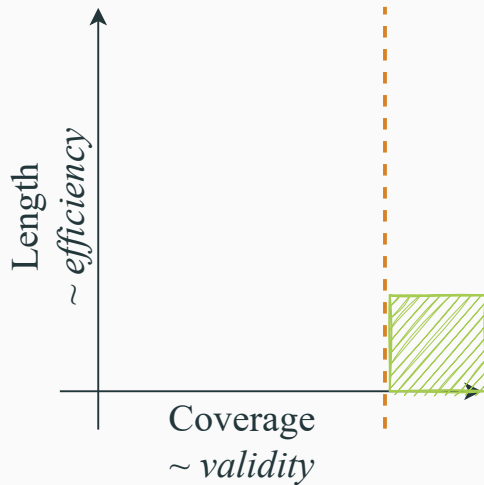
where the $X_{t,\cdot} \sim \mathcal{U}([0, 1])$ and ε_t is an ARMA(1,1) process:

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

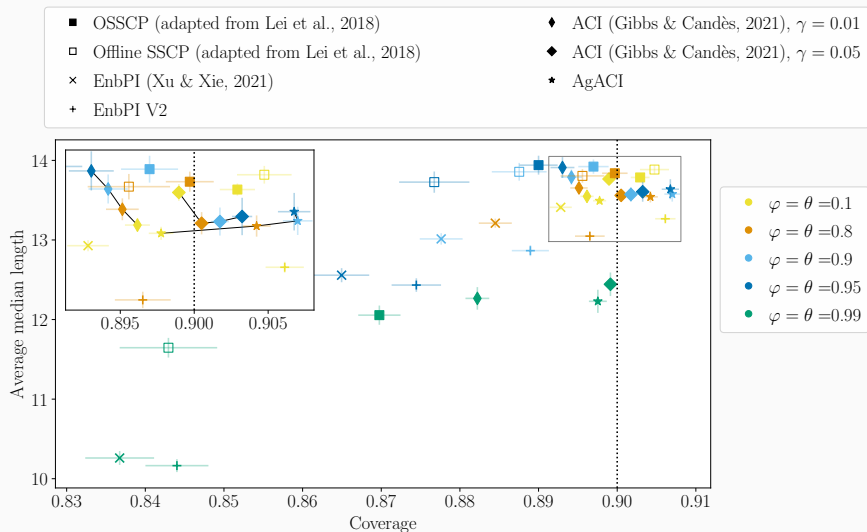
with ξ_t is a white noise of variance σ^2 .

- $\varphi = \theta$ range in $[0.1, 0.8, 0.9, 0.95, 0.99]$.
- We fix σ to keep the variance $\text{Var}(\varepsilon_t)$ 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



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*.

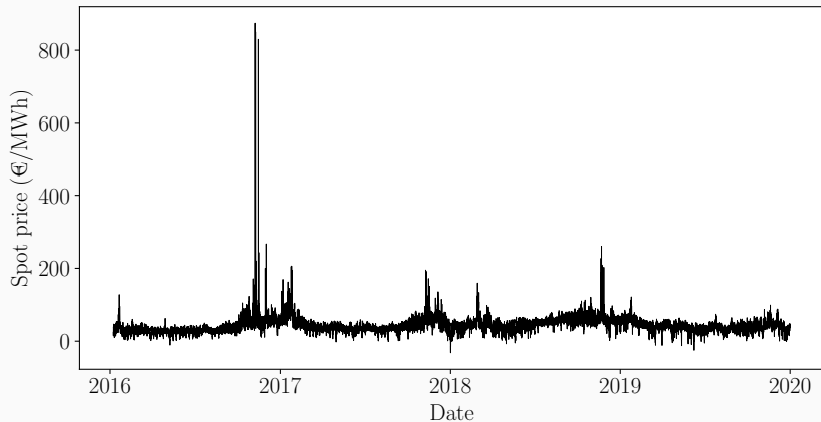


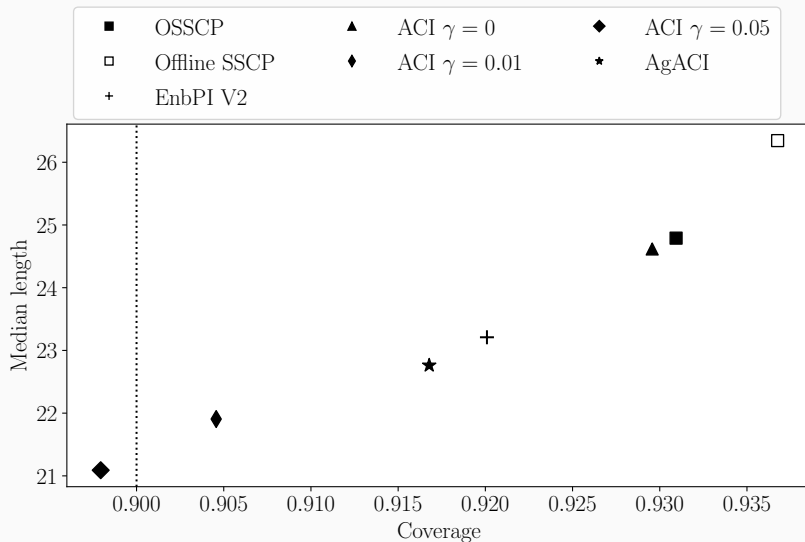
Figure 7: Representation of the French electricity spot price, from 2016 to 2019.

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

↪ 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

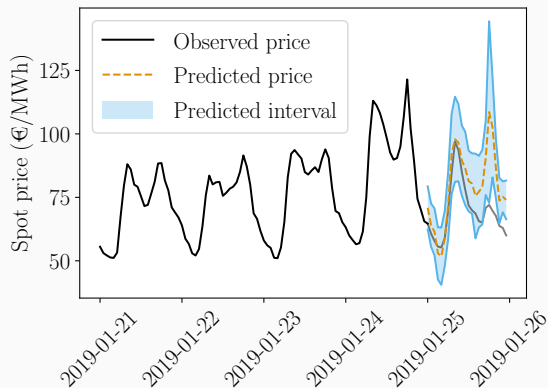


Figure 8: French electricity spot price, its **prediction** and its **uncertainty** with AgACI.

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- 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

- 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

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)
- Ryan Tibshirani [introductive lecture's notes](#)
- [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., Melliush, 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.