Lecture on Conformal Prediction

Margaux Zaffran

December 1-5, 2025

ECAS-SFdS School

Yesterday's lecture

1. On exchangeability (theory)
2. Split conformal prediction (methods) (theory)

Achievable definition of distribution-free validity

$\widehat{C}_\alpha$ = estimated predictive set based on n data points.

Definition (Distribution-free validity)**.**

$\widehat{C}_\alpha$ achieves distribution-free validity if:

- for any distribution $\mathcal{D}$,
- for any associated exchangeable joint distribution $\mathcal{D}^{\text{exch}(n+1)}$,

we have that:

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

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

Split Conformal Prediction: summary

- **Simple** procedure which quantifies the uncertainty of **any** predictive model $\hat{A}$ by returning predictive regions
- **Finite-sample** guarantees
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$\hookrightarrow$ marginal also over the whole calibration set and the test point!

On the design choices of conformity scores and (empirical) conditional guarantees

- Impact of the calibration set on the coverage
- On distribution-free X-conditional validity
- Y-conditional validity
- Case study: healthcare

Beyond exchangeability

SCP: what choices for the regression scores?

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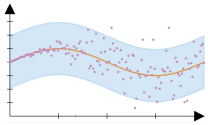
$\mathrm{s}(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$		
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$		
Visu.			
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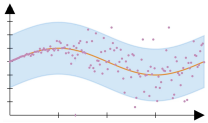
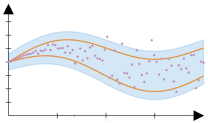
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$		$[\widehat{\mathrm{QR}}_{\mathrm{lower}}(x) - q_{1-\alpha}(\mathcal{S});$ $\widehat{\mathrm{QR}}_{\mathrm{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
Visu.			
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$\mathrm{s}(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$	$\frac{\lvert\hat{\mu}(X) - Y\rvert}{\hat{\rho}(X)}$	$\max(\widehat{\mathrm{QR}}_{\mathrm{lower}}(X) - Y,$ $Y - \widehat{\mathrm{QR}}_{\mathrm{upper}}(X))$
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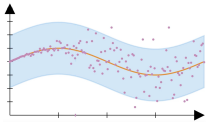
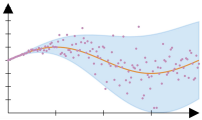
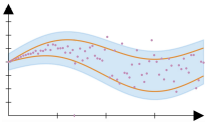
Visu.			
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Challenges that we are going to explore in the today's lecture

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2. Split conformal prediction (methods) (theory)

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4. Beyond exchangeability (methods) (case studies)

Theorem (Distribution conditional on the calibration data)**.**

If the scores are a.s. distinct, SCP outputs $\widehat{C}_\alpha$ such that for any distribution $\mathcal{D}$:

$$\mathbb{P}_{\mathcal{D}}\left(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) | (X_i, Y_i)_{i\in \mathrm{Cal}}\right) \sim \beta\left(k_\alpha, \#\mathrm{Cal} + 1 - k_\alpha\right),$$

with $k_\alpha = \lceil (1-\alpha)(\#\mathrm{Cal}+1) \rceil$.

From the β distribution, we get that it has

expectation $\dfrac{k_\alpha}{k_\alpha + \#\mathrm{Cal} + 1 - k_\alpha} = \dfrac{k_\alpha}{\#\mathrm{Cal}+1} = \dfrac{\lceil (1-\alpha)(\#\mathrm{Cal}+1) \rceil}{\#\mathrm{Cal}+1} \geq 1-\alpha,$

and variance $\dfrac{k_\alpha\left(\#\mathrm{Cal} + 1 - k_\alpha\right)}{\left(\#\mathrm{Cal}+1\right)^2\left(\#\mathrm{Cal}+2\right)} \approx \dfrac{\alpha(1-\alpha)}{\#\mathrm{Cal}+2}.$

Probably Approximately Correct bounds on calibration-conditional coverage (Vovk, 2012; Bian and Barber, 2023)

Theorem (calibration conditional validity of SCP).

SCP outputs $\widehat{C}_\alpha$ such that for any distribution $\mathcal{D}$ and any $0 < \delta \leq 0.5$:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(\mathbb{P}_{\mathcal{D}}\left(Y_{n+1} \notin \widehat{C}_{n,\alpha}(X_{n+1}) \,|\, (X_i, Y_i)_{i=1}^n\right) \leq \alpha + \sqrt{\frac{\log(1/\delta)}{2\#\mathrm{Cal}}}\right) \geq 1-\delta.$$

$\hookrightarrow$ controls the deviation of miscoverage with respect to the nominal level of a predictive set built on a given calibration set.

On the design choices of conformity scores and (empirical) conditional guarantees

- Impact of the calibration set on the coverage
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- Y-conditional validity
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$$\mathbb{P}_{\mathcal{D}^{\text{exch}(n+1)}}\left(Y_{n+1} \in \widehat{C}_\alpha\left(X_{n+1}\right) | X_{n+1}\right) \overset{a.s.}{\geq} 1-\alpha.$$

Informative conditional coverage as such is impossible

Theorem (Impossibility results Vovk (2012); Lei and Wasserman (2014)).

If $\widehat{C}_\alpha$ is distribution-free X-conditionally valid, then, for any $\mathcal{D}$, for $\mathcal{D}_X$–almost all $\mathcal{D}_X$–non-atoms $x \in \mathcal{X}$, it holds:

- *Regression:* $\mathbb{P}_{\mathcal{D}^{\otimes(n)}}\left(\text{mes}\left(\widehat{C}_\alpha(x)\right) = \infty\right) \geq 1 - \alpha$,
- *Classification:* for any $y \in \mathcal{Y}$, $\mathbb{P}_{\mathcal{D}^{\otimes(n)}}\left(y \in \widehat{C}_\alpha(x)\right) \geq 1 - \alpha$.

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Example (Naive estimator).

$\mathcal{C}_\alpha(\cdot; \xi) \equiv \mathcal{Y}\mathbb{1}\{\xi \leq 1 - \alpha\} + \emptyset\mathbb{1}\{\xi > \alpha\}$, where $\xi \sim \mathcal{U}([0, 1])$.

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$\hookrightarrow$ the lower bounds are tight

$\hookrightarrow$ Classification: *every label* is likely to be included in $\widehat{C}_\alpha$.
$\widehat{C}_\alpha$ is likely to be large: for any $\mathcal{D}$, for $\mathcal{D}_X$–almost all $\mathcal{D}_X$–non-atoms $x \in \mathcal{X}$, $\mathbb{E}_{\mathcal{D}^{\otimes(n)}}\left[\#\widehat{C}_\alpha(x)\right] \geq (1-\alpha)\#\mathcal{Y}$.

Getting closer to X-conditional coverage

	X-conditionally valid	
"Non smooth" distribution		

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- 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.

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- Approximate conditional coverage
  $\hookrightarrow$ Romano et al. (2020); Guan (2022); Jung et al. (2023); Gibbs et al. (2023)
  Target $\mathbb{P}(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right) | X^{(n+1)} \in \mathcal{R}(x)) \geq 1 - \alpha$

Non exhaustive references.

Weaker notion of X-conditional validity (Barber et al., 2021)

Definition (distribution-free $(1-\alpha, \delta)$–X-conditional validity)**.**

Let $\delta > 0$ be a tolerance level.

An estimator $\widehat{C}_\alpha$ achieves distribution-free $(1-\alpha, \delta)$–X-conditional validity if for any distribution $\mathcal{D}$, for any $\mathcal{X} \subseteq \mathcal{X}$ such that $\mathbb{P}_{\mathcal{D}_X}(X \in \mathcal{X}) \geq \delta$, and for any associated exchangeable joint distribution $\mathcal{D}^{\text{exch}(n+1)}$, we have:

$$\mathbb{P}_{\mathcal{D}^{\text{exch}(n+1)}}\left(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) \,|\, X_{n+1} \in \mathcal{X}\right) \geq 1-\alpha.$$

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Informal theorem (lower bound on $(1-\alpha, \delta)$–X-cond. valid efficiency)

An estimator achieving $(1-\alpha, \delta)$–X-conditional validity can not be more efficient than an estimator achieving **distribution-free marginal validity at the level** $1-\alpha\delta$.

$\hookrightarrow$ In practive, consider small $\delta \rightarrow$ unefficient predictive sets.

Pre-defined partition of the $\mathcal{X}$ space

$\widehat{C}_\alpha$ = estimated predictive set based on n data points.

$\mathcal{G}$ a set of "groups" (i.e., define G a random variable taking its values in $\mathcal{G}$).

Definition (Distribution-free $\mathcal{G}$-conditional validity ($\mathcal{G}$CV)).

$\widehat{C}_\alpha$ achieves distribution-free $\mathcal{G}$-conditional validity if for any distribution $\mathcal{D}$ on $(\mathcal{X}, \mathcal{G}, \mathcal{Y})$, it holds that:

$$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}, G^{(n+1)}\right) | G^{(n+1)}\right) \overset{a.s.}{\geq} 1-\alpha.$$

Theorem (General $\mathcal{G}$CV hardness result).

If $\widehat{C}_\alpha$ is distribution-free $\mathcal{G}$-conditionally valid then for any distribution $\mathcal{D}$, for any group g such that $\mathcal{D}_G(g) := \mathbb{P}_{\mathcal{D}}(G = g) > 0$, it holds:

- *Regression*

  $$\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(\text{mes}\left(\widehat{C}_\alpha\left(X_{n+1}, g\right)\right) = \infty\right) \geq 1 - \alpha - \Delta_{g,n} \geq 1 - \alpha - \mathcal{D}_G(g)\sqrt{n+1},$$

- *Classification*

  for any $y \in \mathcal{Y}$, $\mathbb{P}_{\mathcal{D}^{\otimes(n+1)}}\left(y \in \widehat{C}_\alpha\left(X_{n+1}, g\right)\right) \geq 1 - \alpha - \Delta_{g,n} \geq 1 - \alpha - \mathcal{D}_G(g)\sqrt{n+1}.$

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Hardness results on G-conditional-validity (Zaffran et al., 2024)

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$\hookrightarrow$ gets negligible (making the lower bound nearly $1 - \alpha$) **only** for low probability groups compared to n.

Restricting the link between G and (X or Y) does not allow informative $\mathcal{G}$CV

Analogous statements are also available for the classification framework.

Theorem ($G \perp\!\!\!\perp X$ hardness result).

If any $\widehat{C}_\alpha$ is $\mathcal{G}$-conditionally valid under $G \perp\!\!\!\perp X$, then for any distribution $\mathcal{D}$ such that $G \perp\!\!\!\perp X$, for any group g such that $\mathcal{D}_G(g) > 0$, it holds:

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Theorem ($Y \perp\!\!\!\perp G \,|X$ hardness result).

If any $\widehat{C}_\alpha$ is G-conditionally-valid under $Y \perp\!\!\!\perp G \,|X$, then for any distribution $\mathcal{D}$ such that $Y \perp\!\!\!\perp G \,|X$, for any group g such that $\frac{1}{\sqrt{2}} \geq \mathcal{D}_G(g) > 0$, it holds:

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$\Rightarrow$ Need to restrict **both** the link between G and X, **as well as** between G and Y.

Analogous statements are also available for the classification framework.

Implications for $\mathcal{G}$CV in practice

	$\mathcal{G}$-conditionally valid even when $G \not\perp\!\!\!\perp (X, Y)$	
"Non smooth" distribution		

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Achieving Y-conditional validity in classification

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 $\mathcal{A}$ on the proper training set* $(X_i, Y_i)_{i \in \mathrm{Tr}}$)
3. **For** any candidate $y \in \mathcal{Y}$:
   On the calibration set, obtain a set of $\#\mathrm{Cal}_y + 1$ conformity scores :
   $$\mathcal{S}_y = \{S_i = \mathsf{s}\left(X_i, y; \hat{A}\right), i \in \mathrm{Cal} \text{ such that } Y_i = y\} \cup \{+\infty\}$$
4. For a new point X_{n+1}, return $\widehat{C}_{n,\alpha}(X_{n+1}) \left\{ y \text{ such that } \mathsf{s}\left(X_{n+1}, y; \hat{A}\right) \leq q_{1-\alpha}(\mathcal{S}_y) \right\}$

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$\hookrightarrow$ What if there is a high class imbalance?

Ding et al. (2023) proposed to instead obtain **cluster**-conditional coverage.

Image to Image regression with DF-UQ – Angelopoulos et al. (2022)

- Medical application
- Image based task
- Pixel by pixel analysis $\rightsquigarrow$ applications to segmentation for self-driving cars

Image-to-Image Regression with Distribution-Free Uncertainty Quantification and Applications in Imaging

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1. **Task**: *Image to Image regression* – for each pixel of an image, predict a real valued output from the entire image.
2. **UQ Goal:** provide a predictive interval for each pixel, such that the output is in the interval at least 90% of the time.

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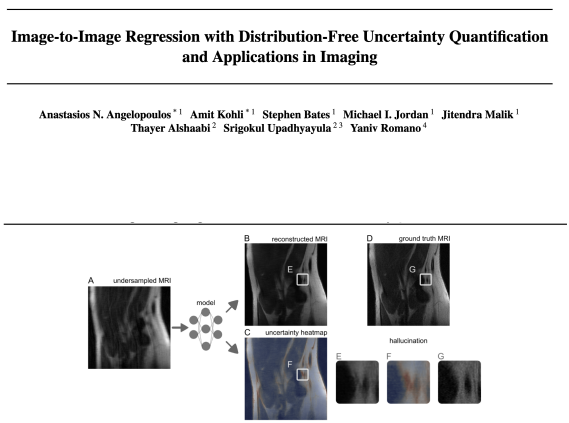

Figure 1. **An algorithmic MRI reconstruction with uncertainty.** A rapidly acquired but undersampled MR image of a knee (A) is fed into a model that predicts a sharp reconstruction (B) with calibrated uncertainty (C). In (C), red means high uncertainty and blue means low uncertainty. Wherever the reconstruction contains hallucinations, the uncertainty is high; see the hallucination in the image patch (E), which has high uncertainty in (F), and does not exist in the ground truth (G). For experimental details, see Section 3.4.

Figure 1: Image from Angelopoulos et al. (2022)

Image to Image regression with DF-UQ – Angelopoulos et al. (2022)

Method:

1. Split conformal prediction method - isolate calibration set
2. On the proper training set, learn:
    - Mean regressor - $\hat{\mu} : \mathbb{R}^{NM} \to [0; 1]$

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$$[\hat{\mu}(X) - \tilde{\ell}(X); \hat{\mu}(X) + \tilde{u}(X)]$$

   $\to$ 3 regressors are used

   4 techniques are experimented for these regressors, including QR.

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Guarantee:

$$\mathbb{P}\left[\mathbb{E}\left[\text{Average miscoverage on all pixels of a test image}|\text{Cal}\right] \geq \alpha\right] \leq \delta$$

$\to$ Marginal validity on the test, with high probability w.r.t. the calibration set.

Image to Image regression with DF-UQ – Angelopoulos et al. (2022)

Abstract

Image-to-image regression is an important learning task, used frequently in biological imaging. Current algorithms, however, do not generally offer statistical guarantees that protect against a model's mistakes and hallucinations. To address this, we develop uncertainty quantification techniques with rigorous statistical guarantees for image-to-image regression problems. In particular, we show how to derive uncertainty intervals around each pixel that are guaranteed to contain the true value with a user-specified confidence probability. Our methods work in conjunction

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We now formally describe the method for constructing uncertainty intervals. Each pixel in the image will get its own uncertainty interval, as in (1), that is statistically guaranteed to contain the true value with high probability.

How do you understand that?

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- Not a conditional coverage claim!
- The statement is on-average on the test point - easy or hard.

Size-stratified risk. Next, we seek prediction sets that do not systematically make mistakes in difficult parts of the image. Our risk control requirement in Definition 2.1 may be satisfied even if the prediction sets systematically fail to contain the most difficult pixels. For example, if $\alpha = 0.1$ and 90% of pixels are covered by fixed-width intervals of size 0.01, then the requirement is satisfied—however, the sets no longer serve as useful notions of uncertainty. To

2. Methods

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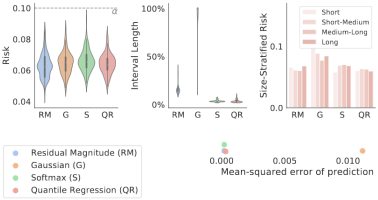
- Hard problem (impossibility results!)
- Introduce metrics to see *if* and *on which underlying regressors* such problem happens.

How do you understand that?

Image to Image regression with DF-UQ – Angelopoulos et al. (2022)

Example of such metrics (see also Feldman et al., 2021) **:**

- Link between the size of the PI and the coverage level $\longrightarrow$



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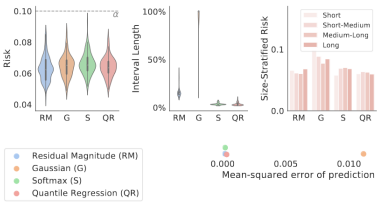

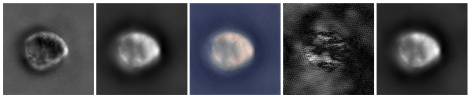

Figure 3. **Examples of quantitative phase reconstructions of leukocytes with uncertainty** shown in the following order: input (we only show one of the two illuminations), prediction, uncertainty visualization (produced with quantile regression), absolute difference between prediction and ground truth (renormalized for visualization), ground truth.

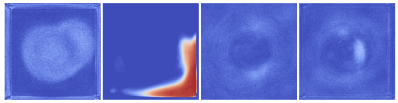

Figure 8. **Spatial variations in miscoverage** in the BSCCM dataset are shown for each of the four methods as a heatmap. Blue represents 0% miscoverage and red represents 100%. The methods are, in order, residual magnitude, gaussian, softmax, and quantile regression.

Figure 2: All images from Angelopoulos et al. (2022)

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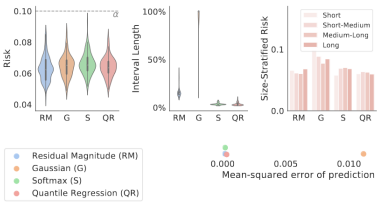

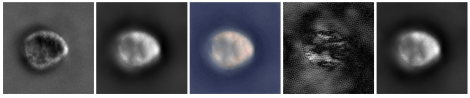

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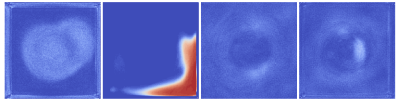

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Take aways:

- Elegant application of SCP with CQR type score
- Test marginal and calibration + train conditional validity guarantees with HP
- Main problem is Test conditionality $\rightarrow$ look at metrics to evaluate which methods performs best!

On the design choices of conformity scores and (empirical) conditional guarantees

Beyond exchangeability

- Some (short) literature review
- Case study: electricity price forecasting

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- ✗ Possibly many shifts, not only one

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Generalizations

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    $\hookrightarrow$ 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
    $$\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})) \geq 1 - \alpha - \underbrace{\text{average violation of exchangeability by each calibration point}}$$
    $\hookrightarrow$ proposed algorithm: reweighting again!
    e.g., in a temporal setting, give higher weights to more recent points.

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Online setting

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$\rightsquigarrow$ More during the case study!

Recent developments (as of late 2023...)

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Non exhaustive references.

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  - Idea: track the previous coverages of the predictive intervals ($\mathbb{1}\{Y_t \in \widehat{C}_\alpha(X_t)\}$)
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- 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

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Case study: electricity price forecasting

Forecasting French spot electricity prices

Hourly day-ahead market prices (between producers and suppliers)

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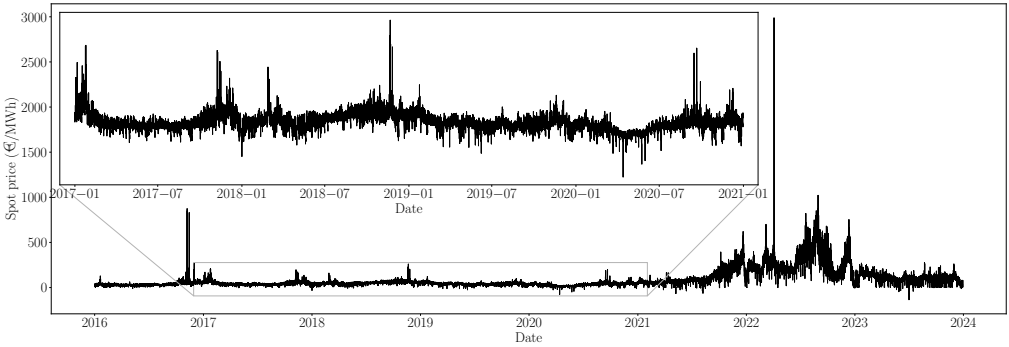

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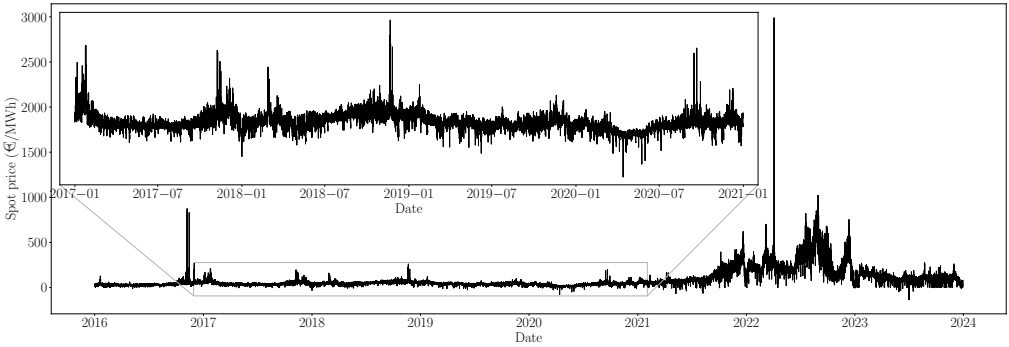
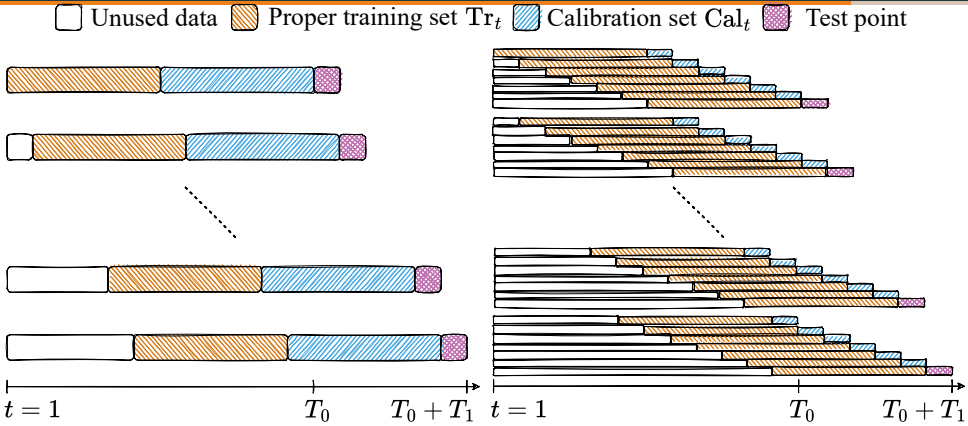


To which extent are they forecastable?

↪ forecasts errors **no lower than 10%** of the realized price!

Temporal splitting strategies: Online Sequential Split Conformal Prediction (OSSCP, Zaffran et al., 2022; Dutot et al., 2024)



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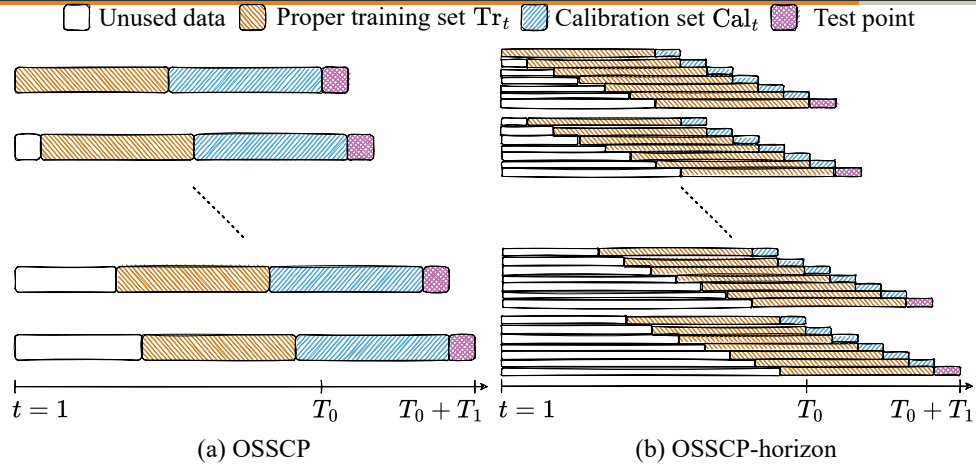

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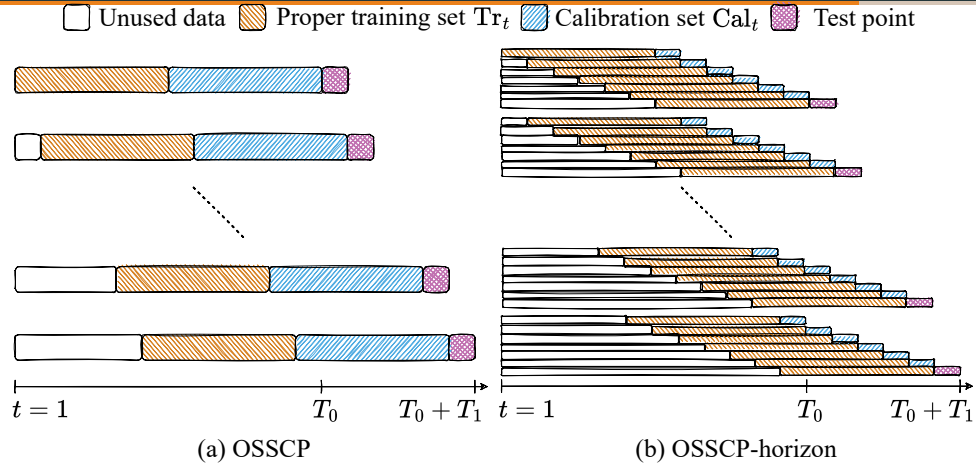

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↪ `OSSCP-horizon` drastically improves robustness in non-stationary temporal settings.

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

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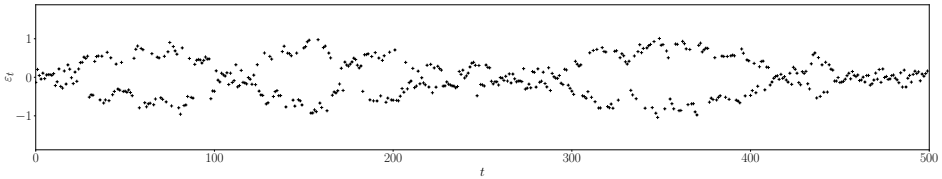
$\Rightarrow$ favors large γ.

Visualisation of ACI procedure



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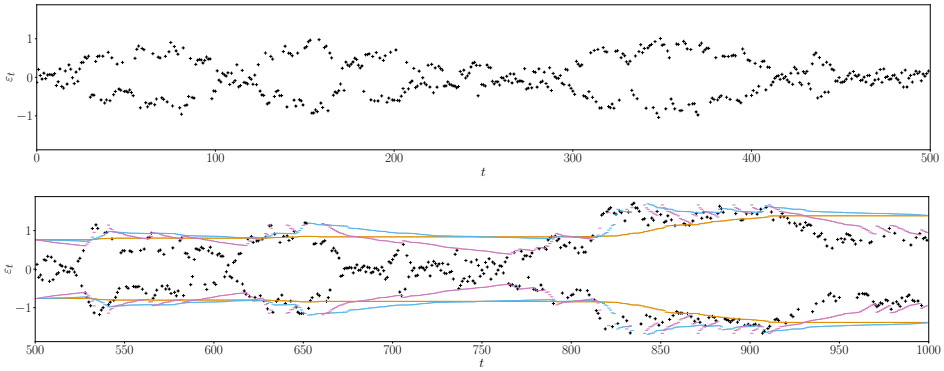
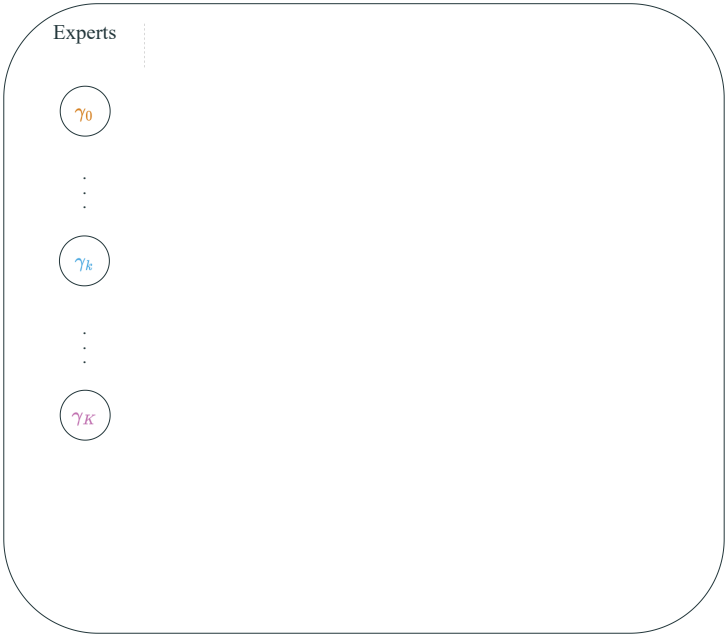


Figure 3: Visualisation of ACI with different values of γ ($\gamma = 0$, $\gamma = 0.01$, $\gamma = 0.05$)

AgACI: adaptive wrapper around ACI, upper bound (Zaffran et al., 2022)



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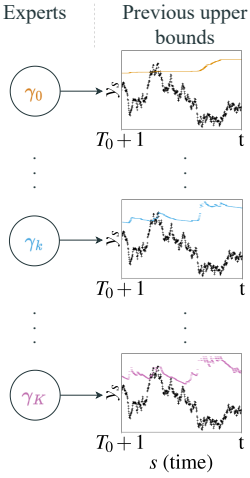

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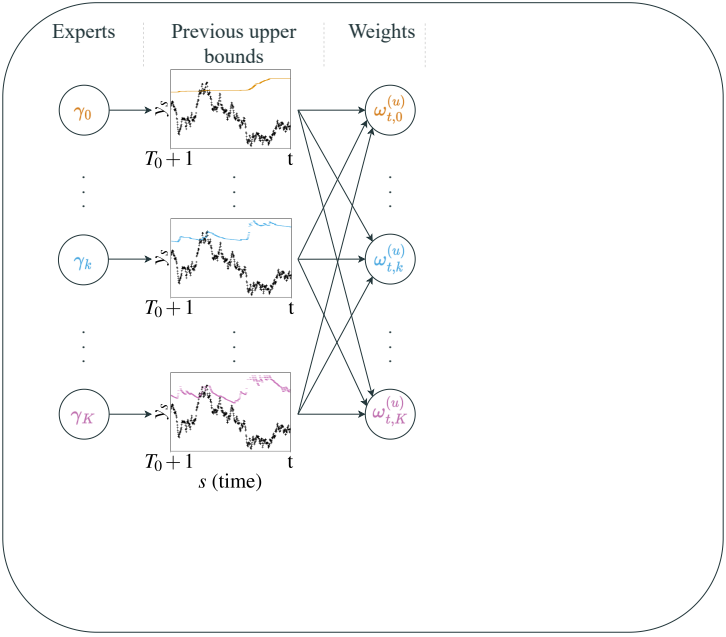

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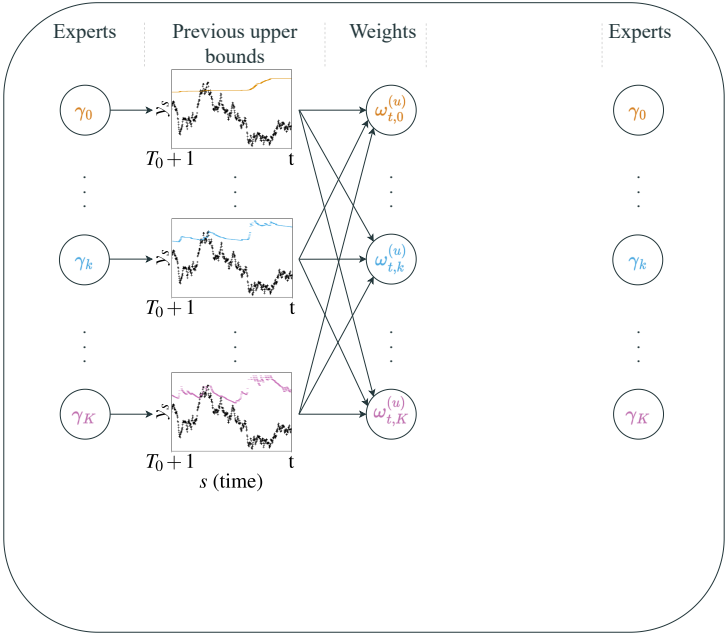

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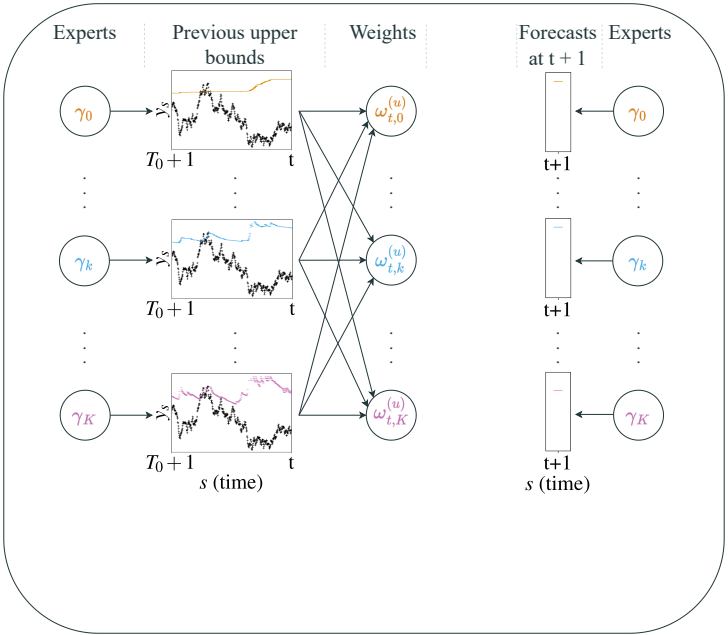

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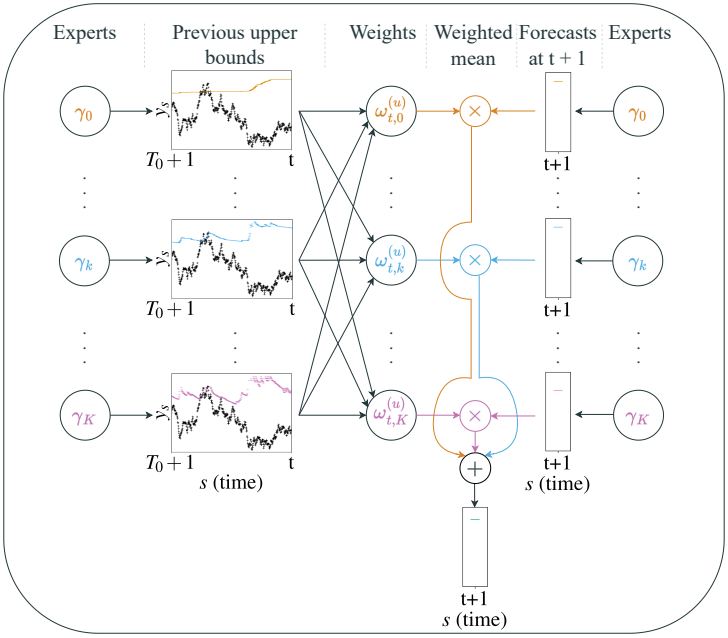
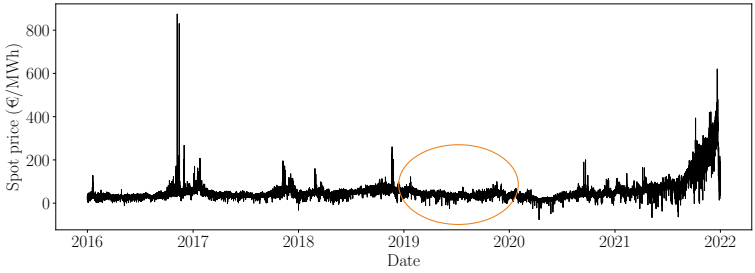


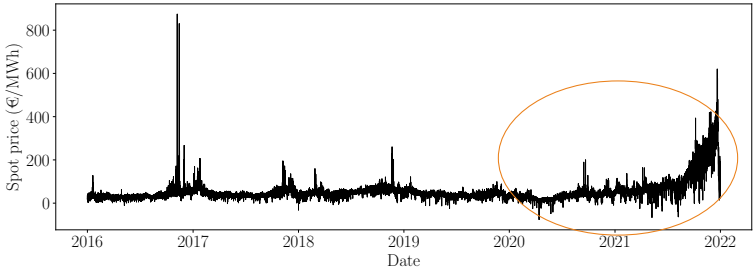
Experimental take-away messages (Zaffran et al., 2022; Dutot et al., 2024)

- 2019: `AgACI` provides validity with a reasonable efficiency;



Experimental take-away messages (Zaffran et al., 2022; Dutot et al., 2024)

- 2019: `AgACI` provides validity with a reasonable efficiency;
- 2020 and 2021: `AgACI` fails to ensure validity, and the various forecasting models considered[1] behave differently.



[1] Quantile Random Forests, Quantile Generalized Additive Models, Quantile Gradient Boosting, etc.

Improving adaptiveness for high non-stationarity (Dutot et al., 2024)

Online aggregation of various `AgACI`, each of them being trained with different underlying forecasting models, for each bound independently.

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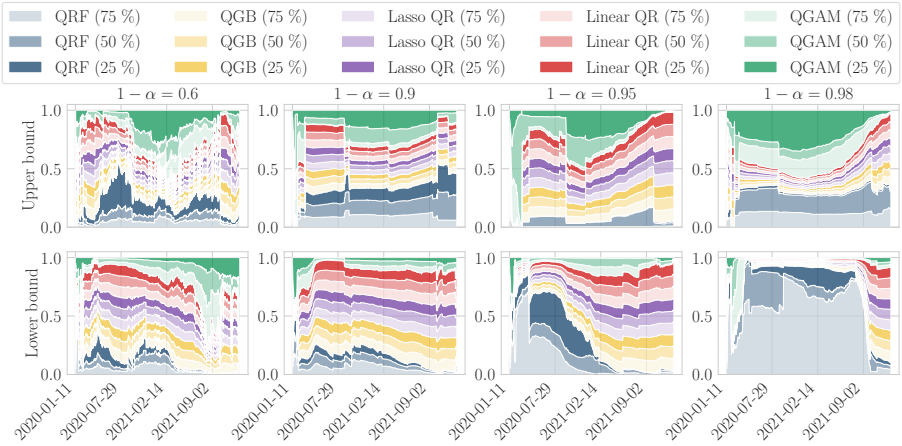

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↪ Weaken the objective and consider a more practical theoretical aim?

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5. Computational and statistical trade-offs (methods) (theory)
6. Handling missing data (methods)

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