

NB: Open with an advanced pdf reader (e.g., Acrobat to have animations)

# Lecture on Conformal Prediction

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Margaux Zaffran

December 1-5, 2025  
ECAS-SFdS School



## Why a lecture on conformal prediction?

- Conformal Prediction comes from the 90s, and has emerged as a popular topic in the early 2020's.
  - 1996-1999: emergence of Conformal Prediction (CP) in the historical machine learning community, by Vladimir Vovk, Alexander Gammerman, Vladimir Vapnik, Glenn Shafer
  - 2012+: Jing Lei, Larry Wasserman and colleagues at Carnegie Mellon University (CMU) bring it to the statistics community
  - 2020+: explosion, notably thanks to Rina Barber, Emmanuel Candès, Aaditya Ramdas and Ryan J. Tibshirani

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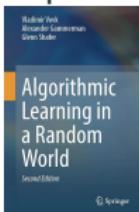
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Successfully applied to
  - Medical applications
  - Markets / demand forecasting
  - Computer Vision

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- Because I believe that conformal methods are **important** tools, whose strengths and limitations are sometimes misunderstood.
- To be part of the **diffusion** effort that many colleagues are making.



Book reference: Vovk et al. (2005)  
(new edition in 2022)



A gentle tutorial: Angelopoulos and Bates (2023)  
+ [Videos playlist](#)



R. J. Tibshirani  
[introductory lecture's notes](#)



Forthcoming book: Angelopoulos, Barber, Bates (2024)  
[arXiv version](#)

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Aymeric Dieuleveut

## Goals

- Provide a detailed introduction to the basics
- Demystify the results: fair introduction with limits
- Give you insights on how to leverage those techniques in your own fields

## Disclaimers

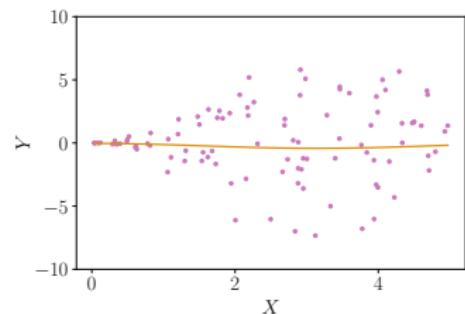
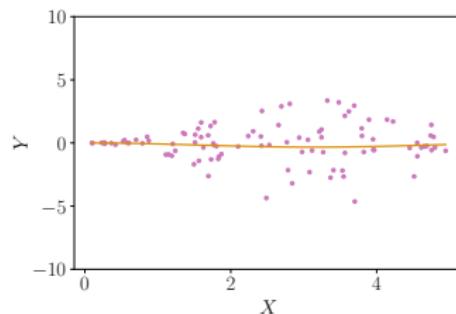
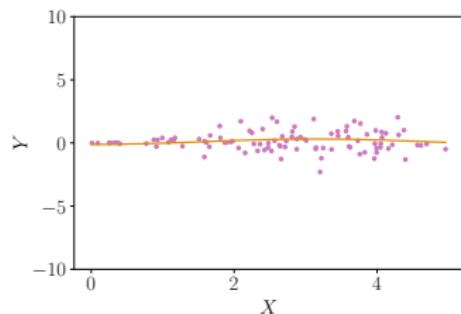
- Many people contributed to the domain - list of references may not be exhaustive
- Multiple other excellent resources

## On the importance of quantifying uncertainty

- **Obvious in most applications - weather, medical, markets**

# On the importance of quantifying uncertainty

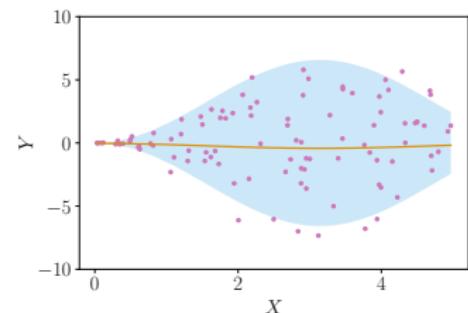
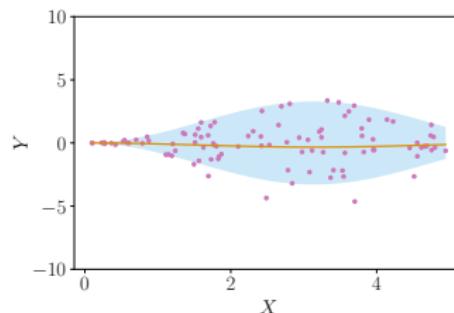
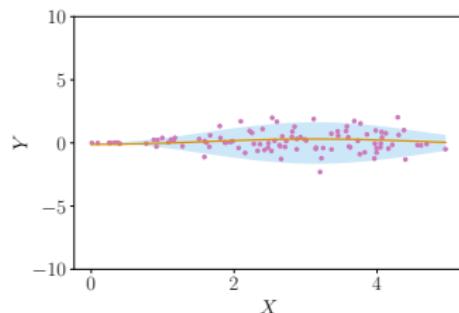
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# On the importance of quantifying uncertainty

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↪ Same “best” predictor, yet 3 distinct underlying phenomena!  
⇒ Quantifying uncertainty conveys this information.

## Introductory remarks

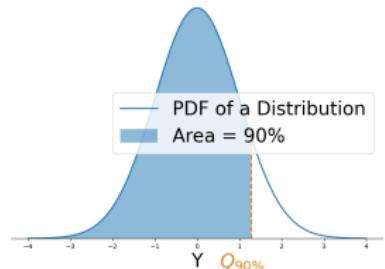
Exchangeability

Split Conformal Prediction (SCP)

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

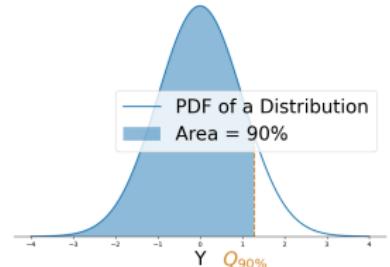
## Reminder about quantiles

- Quantile level  $\beta \in [0, 1]$
- $Q_Y(\beta) := \inf\{t \in \mathbb{R}, \mathbb{P}(Y \leq t) \geq \beta\}$



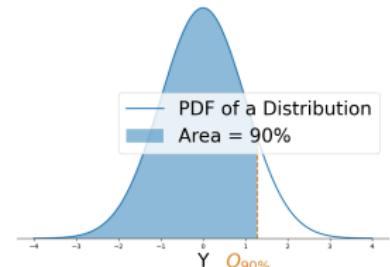
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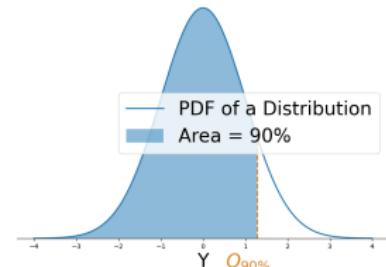


↪ Defining the **order statistics** of a random vector  $(Y_1, \dots, Y_n)$  by  
 $(Y_{(1)}, \dots, Y_{(n)})$ , with  $Y_{(1)} \leq \dots \leq Y_{(n)}$ , we have:

$$q_\beta(Y_1, \dots, Y_n) = Y_{(\lceil \beta \times n \rceil)}$$

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**Example** (a special quantile: the median).

$$\beta = 0.5$$

↪  $q_{0.5}(Y_1, \dots, Y_n)$  is the empirical median of  $(Y_1, \dots, Y_n)$ ;

↪  $Q_Y(0.5)$  represents the median of the distribution of  $Y$ .

↪  $Q_Y(0.5) = \arg \min_c \mathbb{E} [|Y - c|]$ .

## Median regression

- The Bayes predictor depends on the chosen loss function.

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

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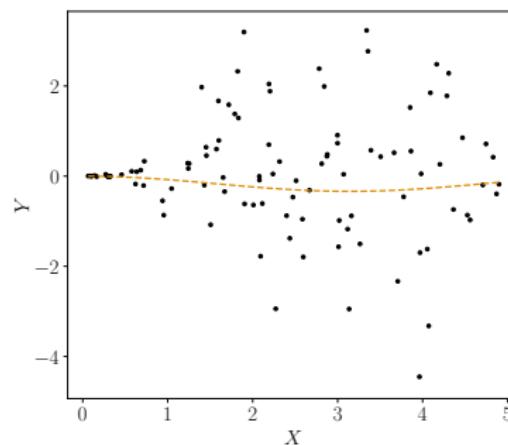
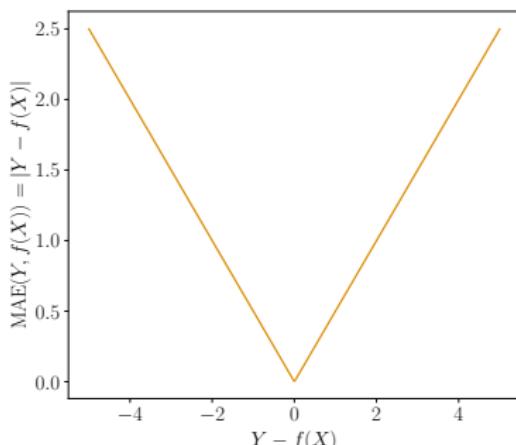
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$$\Rightarrow f^*(X) = \operatorname{median}[Y|X] = Q_{Y|X}(0.5)$$



## Generalization: Quantile regression

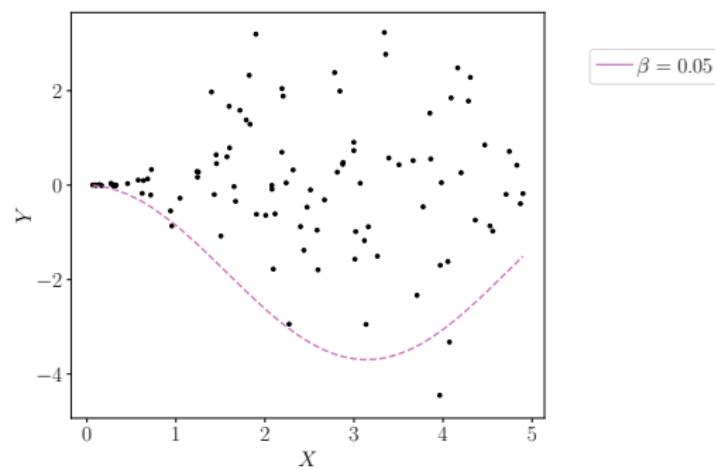
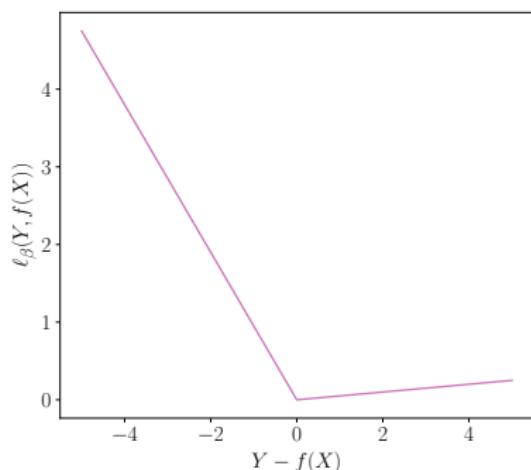
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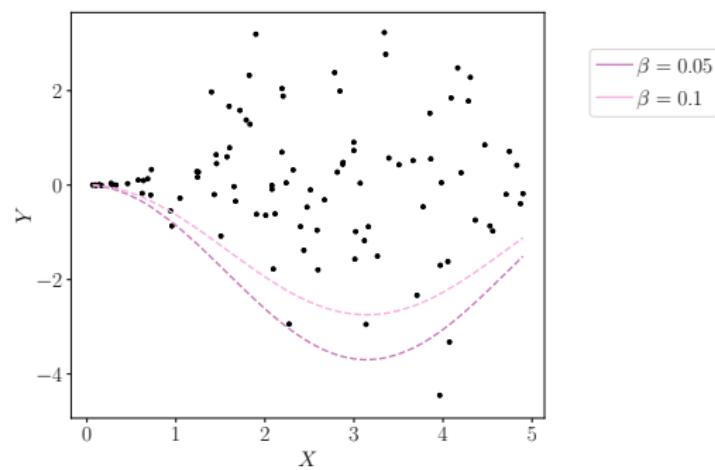
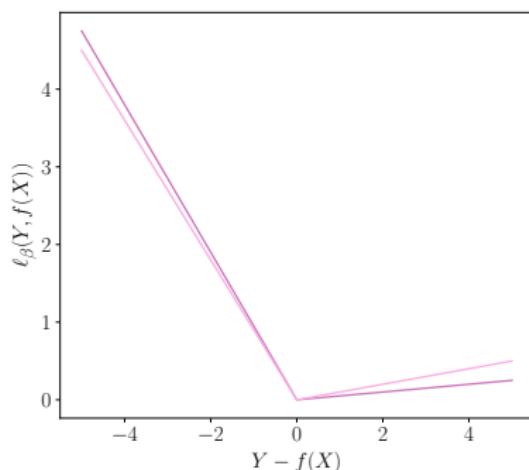
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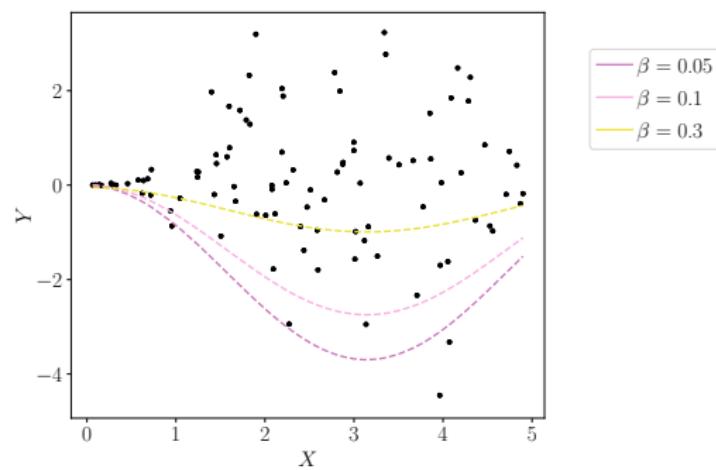
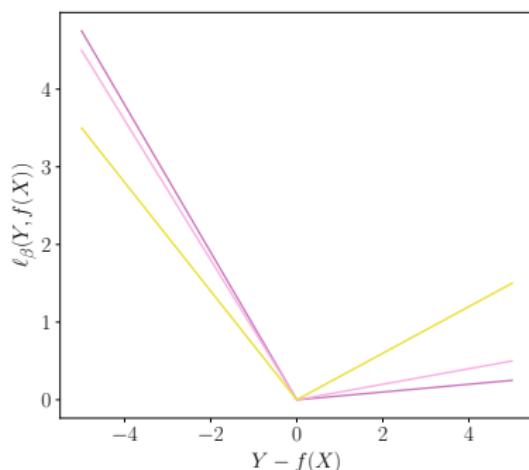
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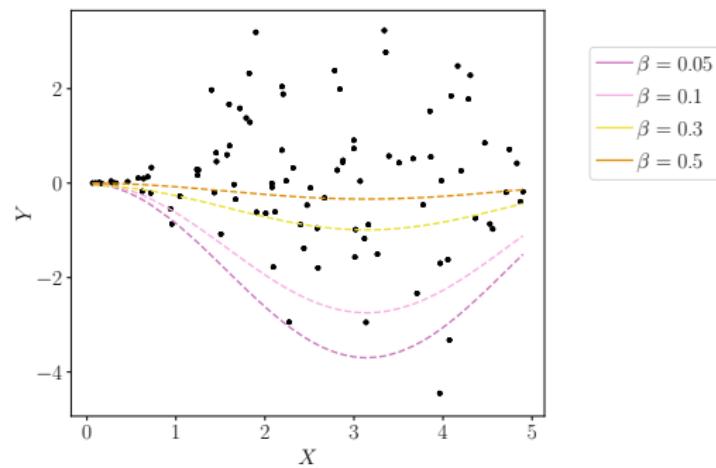
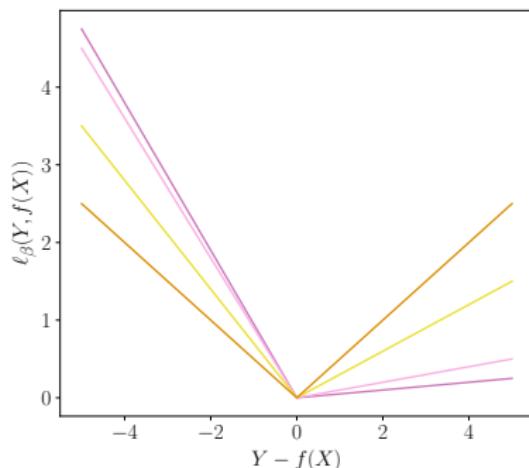
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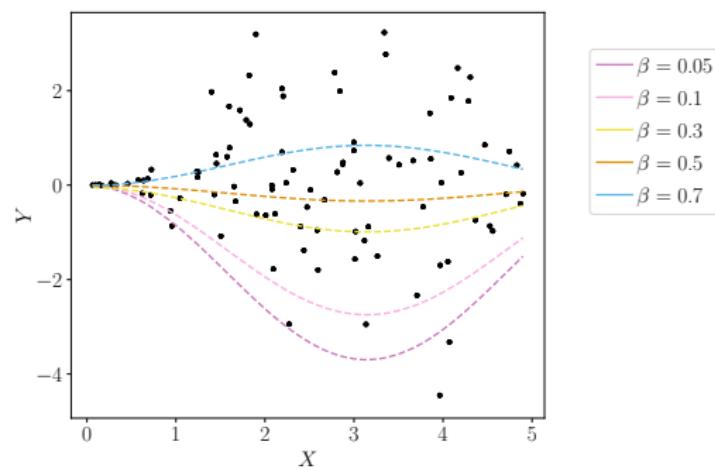
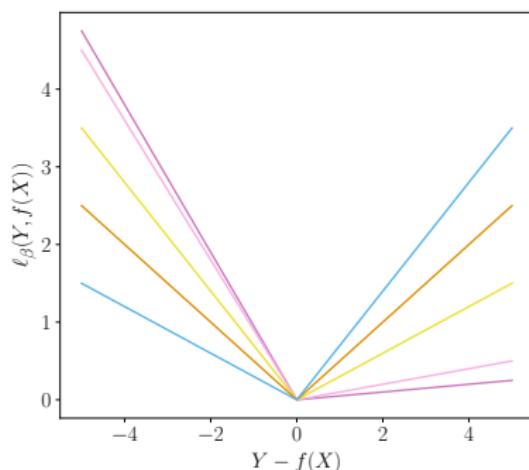
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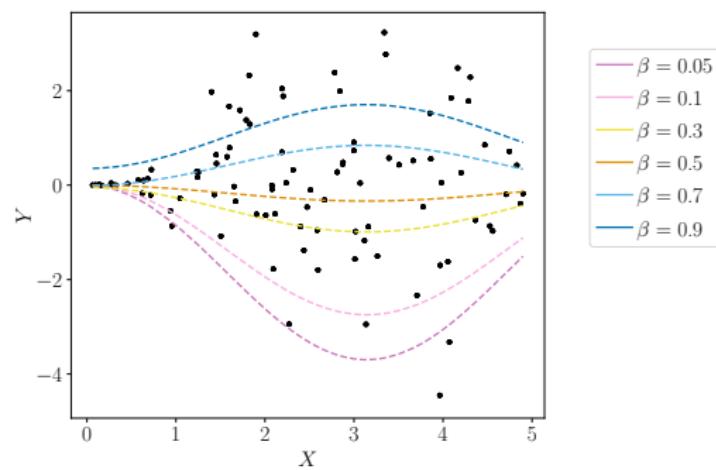
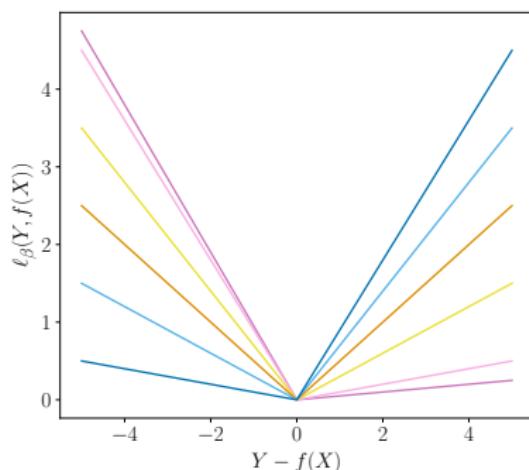
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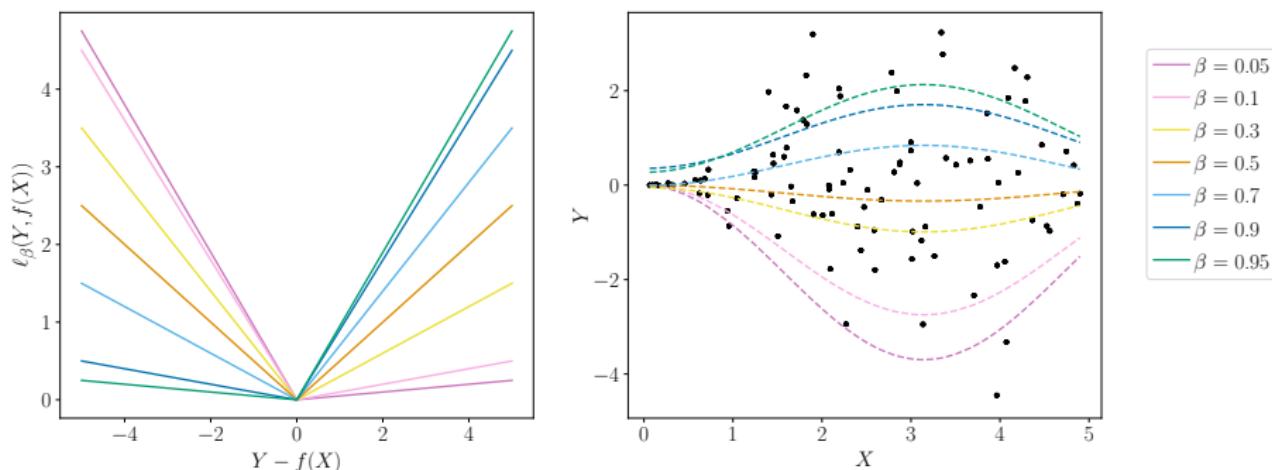
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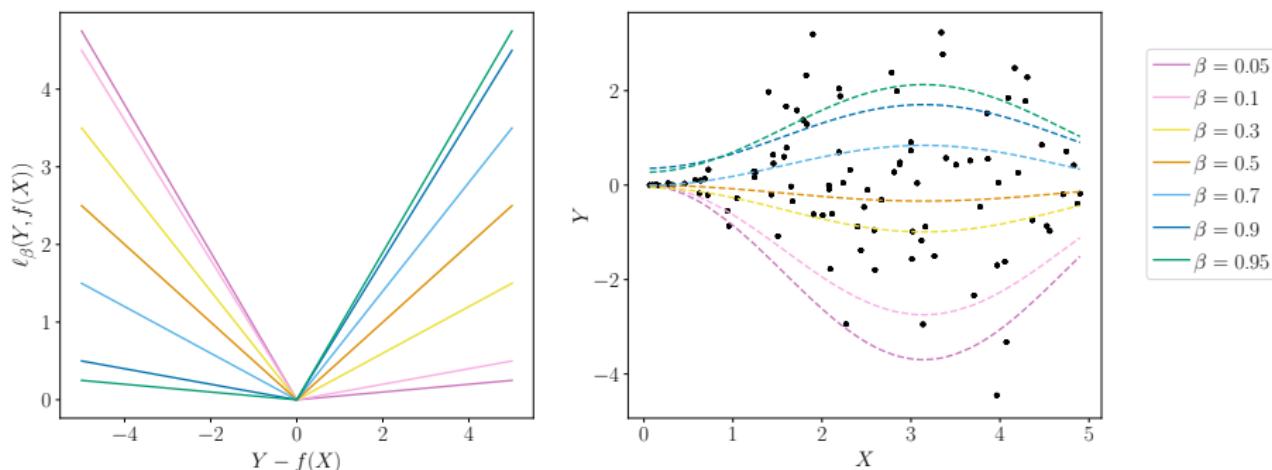
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## Quantifying predictive uncertainty

- $(X, Y) \in \mathcal{X} \times \mathcal{Y}$  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:

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

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

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### Post-hoc design (black-box view)

We aim for an approach that works in a post-hoc fashion on top of *any*  $\mathcal{A}$ , with no impact of the choice of  $\mathcal{A}$  on the validity of the method.

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- Construction of the predictive intervals should be
  - agnostic to the model
  - agnostic to the data distribution
- Validity should be ensured
  - in finite samples
  - for all data distribution and underlying model

## Attempt to define distribution-free validity

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

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

$\widehat{C}_\alpha$  achieves (lofty) distribution-free validity if for any joint distribution  $\mathcal{D}_{n+1}$  on  $(\mathcal{X} \times \mathcal{Y})^{n+1}$ , we have that:

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- ♥ In fact, we can even weaken this to exchangeable distributions.

# This is what we are jumping into!

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1. On exchangeability (theory)
2. Split conformal prediction (theory)
3. Towards conditional coverage? (theory)
4. Beyond exchangeability
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5. Computational and statistical trade-offs (methods) (theory)
6. Handling missing data (methods)

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1. On exchangeability (theory)
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Exchangeability

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**Definition** (Exchangeability).

$(Z_i)_{i=1}^n$ , a random vector taking values in  $\mathcal{Z}^n$ , is **exchangeable** if, for any permutation  $\sigma$  of  $\llbracket 1, n \rrbracket$ :

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In particular, exchangeability implies that all the entries of  $(Z_i)_{i=1}^n$  are identically distributed.

**Example** (exchangeable sequences).

- $Z_1, \dots, Z_n \stackrel{i.i.d.}{\sim} \mathcal{D}$

## Some examples of exchangeable random vectors

**Example** (exchangeable sequences).

- $Z_1, \dots, Z_n \stackrel{i.i.d.}{\sim} \mathcal{D}$

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

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- Sampling without replacement from  $\{z_1, \dots, z_n\}$

### Characterization in a countable space

Denote  $p$  the probability mass function of the joint distribution of  $(Z_1, \dots, Z_n)$ .

$(Z_1, \dots, Z_n)$  are exchangeable if and only if, for any permutation  $\sigma$  of  $\llbracket 1, n \rrbracket$ , for any  $(z_1, \dots, z_n) \in \mathcal{Z}^n$  we have:

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### Characterization in a continuous space

Assume  $(Z_1, \dots, Z_n)$  admits a probability density function, denoted  $f$ .

$(Z_1, \dots, Z_n)$  are exchangeable if and only if, for any permutation  $\sigma$  of  $\llbracket 1, n \rrbracket$ , for almost any  $(z_1, \dots, z_n) \in \mathcal{Z}^n$  we have:

$$f(z_1, \dots, z_n) = f(z_{\sigma(1)}, \dots, z_{\sigma(n)}).$$

Blackboard time!

$\widehat{C}_\alpha$  = 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:

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

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## SCP: theoretical guarantees

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

**Theorem** (Marginal validity).

Suppose  $(X_i, Y_i)_{i=1}^{n+1}$  are exchangeable<sup>a</sup>. SCP applied on  $(X_i, Y_i)_{i=1}^n$  outputs  $\widehat{C}_\alpha(\cdot)$  such that:

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

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

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<sup>a</sup>Only the calibration and test data need to be exchangeable.

## Proof architecture of SCP guarantees

Blackboard time!

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

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- ✓ Distribution free, model (regressor) free, finite sample average validity guarantee.

## Standard mean-regression SCP – strength: validity – good vs bad estimator

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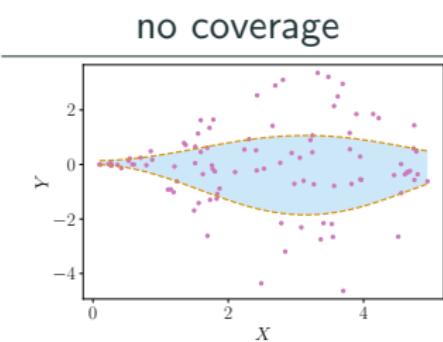
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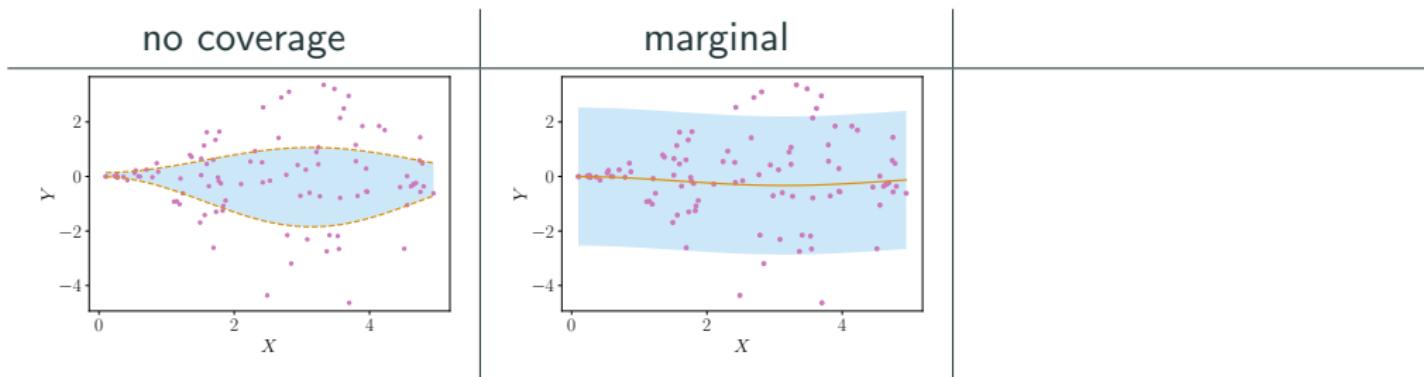
- ✗ Marginal coverage:  $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) \mid X_{n+1} = x\right\} \geq 1 - \alpha$

## Conditional coverage implies adaptiveness



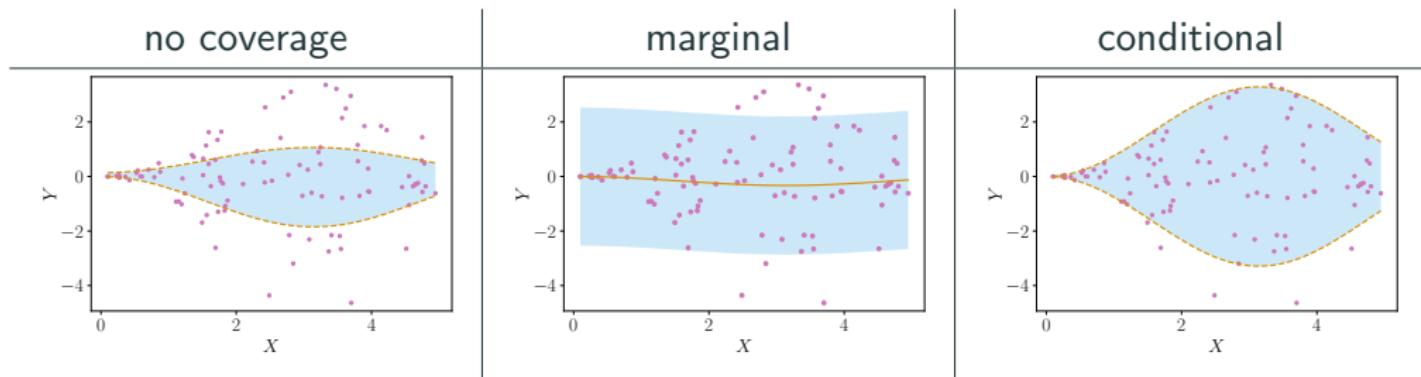
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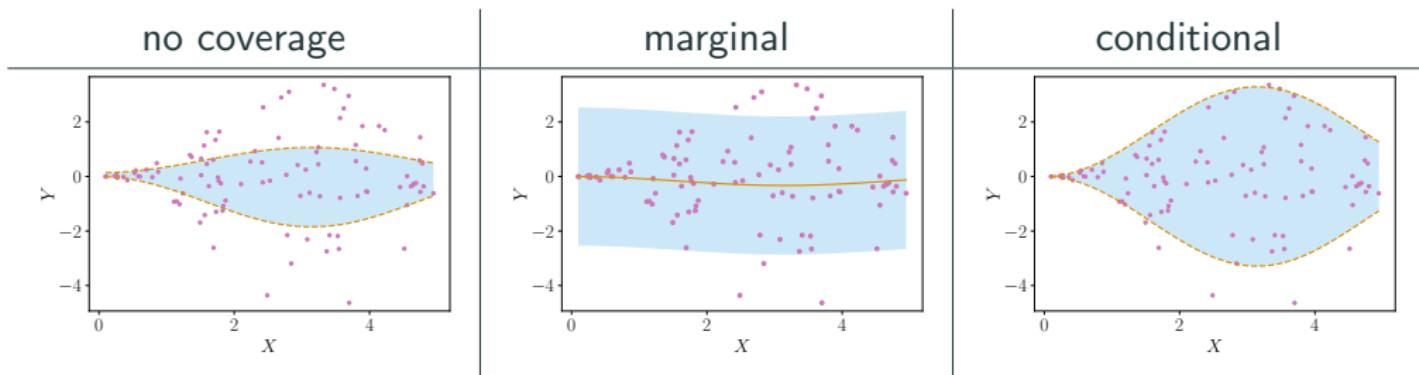
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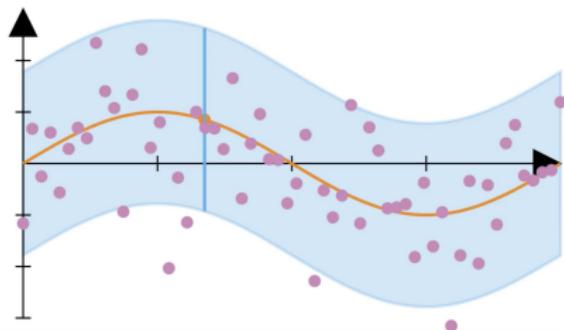


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- Conditional coverage is **stronger** than marginal coverage



## Standard mean-regression SCP – weakness: not adaptive



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

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## Conformalized Quantile Regression (CQR) (Romano et al., 2019)

## CQR: under vs over coverage



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Proof: blackboard!

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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**

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

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

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

4. Compute the  $1 - \alpha$  quantile of these scores, noted  $q_{1-\alpha}(\mathcal{S})$

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5. For a new point  $X_{n+1}$ , return

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

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

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Ex 2:  $\widehat{C}_\alpha(X_{n+1}) = [\widehat{QR}_{\text{lower}}(X_{n+1}) - q_{1-\alpha}(\mathcal{S});$   
 $\widehat{QR}_{\text{upper}}(X_{n+1}) + q_{1-\alpha}(\mathcal{S})]$

## SCP is defined by the conformity score function



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→ 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** (Marginal validity of SCP Vovk et al. (2005)).

Suppose  $(X_i, Y_i)_{i=1}^{n+1}$  are exchangeable<sup>a</sup>. 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  $\{S_i\}_{i \in \text{Cal}} \cup \{S_{n+1}\}$  are almost surely distinct, then

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

---

<sup>a</sup>Only the calibration and test data need to be exchangeable.

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<sup>a</sup>Only the calibration and test data need to be exchangeable.

Proof: application of the quantile lemma.

## SCP: theoretical guarantees

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

**Theorem** (Marginal validity of SCP Vovk et al. (2005)).

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---

<sup>a</sup>Only the calibration and test data need to be exchangeable.

Proof: application of the quantile lemma.

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

Introductory remarks

Exchangeability

## **Split Conformal Prediction (SCP)**

Standard regression case

Conformalized Quantile Regression (CQR)

Generalization of SCP: going beyond regression

**Some examples of classification scores**

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

- $Y \in \{1, \dots, C\}$  ( $C$  classes)
- $\hat{A}(X) = (\hat{p}_1(X), \dots, \hat{p}_C(X))$  (estimated probabilities)

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

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

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$S_i$	0.05	0.1	0.15	0.40	0.45	0.50	0.55	0.55	0.6	0.65

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- $q_{1-\alpha}(\mathcal{S}) = 0.65$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

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

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

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

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

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

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

- Scores on the calibration set

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- $q_{1-\alpha}(\mathcal{S}) = 0.65$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, \mathbf{0.35})$

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

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

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

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

$$\hookrightarrow s(\hat{A}(X_{n+1}), \text{"cat"}) = 0.65 \leq q_{1-\alpha}(\mathcal{S})$$

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

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

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

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

- Scores on the calibration set

$\text{Cal}_i$	"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

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

## SCP: standard classification in practice, cont'd

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

- Scores on the calibration set

Cal <sub>i</sub>	"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
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$S_i$	0.05	0.1	0.15	0.15	0.20	0.25	0.30	0.35	0.40	0.45

- $q_{1-\alpha}(\mathcal{S}) = 0.45$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

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

$$\hookrightarrow s(\hat{A}(X_{n+1}), \text{"tiger"}) = 0.40$$

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

## SCP: standard classification in practice, cont'd

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

- Scores on the calibration set

Cal <sub>i</sub>	"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
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- $q_{1-\alpha}(\mathcal{S}) = 0.45$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

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

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

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

## SCP: standard classification in practice, cont'd

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

- Scores on the calibration set

Cal <sub>i</sub>	"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
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$S_i$	0.05	0.1	0.15	0.15	0.20	0.25	0.30	0.35	0.40	0.45

- $q_{1-\alpha}(\mathcal{S}) = 0.45$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

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

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

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

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

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

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

## SCP: standard classification in practice, cont'd

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

- Scores on the calibration set

Cal <sub>i</sub>	"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
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$\hat{p}_{\text{cat}}(X_i)$	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

- $q_{1-\alpha}(\mathcal{S}) = 0.45$
- $\hat{A}(X_{n+1}) = (0.05, 0.60, 0.35)$

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

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

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

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

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

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

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

### Efficiency yet non-adaptivity of the simplest classification scores

- ✓ Outputs the most efficient set possible (i.e. achieving the smallest average set size, Sadinle et al., 2018),
- ✗ Does not allow to discriminate between “easy” and “hard” test point.  
In practice, it leads to predictive sets that under-cover (resp. over-cover) on “hard” (resp. “easy”) subgroups.  
This is due to the fact that only the prediction for the true class is used to construct the scores.

## SCP: classification with Adaptive Prediction Sets<sup>8</sup>

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1. Sort in decreasing order  $\hat{p}_{\sigma_x(1)}(x) \geq \dots \geq \hat{p}_{\sigma_x(C)}(x)$

---

<sup>8</sup>Romano et al. (2020), *Classification with Valid and Adaptive Coverage*, NeurIPS

## SCP: classification with Adaptive Prediction Sets<sup>8</sup>

1. Sort in decreasing order  $\hat{p}_{\sigma_x(1)}(x) \geq \dots \geq \hat{p}_{\sigma_x(C)}(x)$
2.  $s(x, y; \hat{p}) := \sum_{k=1}^{\sigma_x^{-1}(y)-1} \hat{p}_{\sigma_x(k)}(x)$  (sum of the estimated probabilities associated to classes at least as large as that of the true class  $Y$ )

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3. Return the set of classes  $\{\sigma_{X_{n+1}}(1), \dots, \sigma_{X_{n+1}}(r^*)\}$ , where  
$$r^* = \arg \max_{1 \leq r \leq C} \left\{ \sum_{k=1}^r \hat{p}_{\sigma_{X_{n+1}}(k)}(X_{n+1}) < q_{1-\alpha}(\mathcal{S}) \right\} + 1$$

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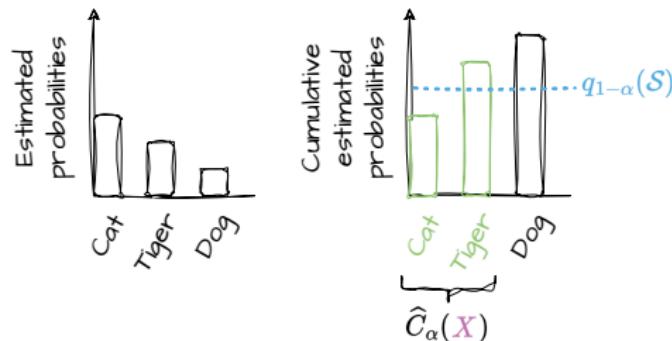
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<sup>8</sup>Romano et al. (2020), *Classification with Valid and Adaptive Coverage*, NeurIPS  
Figure highly inspired by Angelopoulos and Bates (2023).

# 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 <sub>i</sub>	"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	0.05	0.10	0.15
$\hat{p}_{\text{tiger}}(X_i)$	0.02	0.05	0.10	0.85	0.80	0.75	0.75	0.50	0.30	0.30
$\hat{p}_{\text{cat}}(X_i)$	0.03	0.05	0.05	0.10	0.15	0.20	0.15	0.45	0.60	0.55
$S_i$	0	0	0	0	0	0	0	0.5	0	0

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- $q_{1-\alpha}(\mathcal{S}) = 0.5$

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$$\rightarrow \text{Ex 1: } \hat{A}(\mathcal{X}_{n+1}) = (0.15, 0.4, 0.45)$$

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- $q_{1-\alpha}(\mathcal{S}) = 0.5$

→ Ex 1:  $\hat{A}(\textcolor{violet}{X}_{n+1}) = (0.15, 0.4, 0.45)$ ,  $r^* = 2$

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

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

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→ Ex 1:  $\hat{A}(\textcolor{violet}{X}_{n+1}) = (0.15, 0.4, 0.45)$ ,  $r^* = 2$

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

→ Ex 2:  $\hat{A}(\textcolor{violet}{X}_{n+1}) = (0.03, 0.95, 0.02)$

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- $q_{1-\alpha}(\mathcal{S}) = 0.5$

→ Ex 1:  $\hat{A}(\textcolor{violet}{X}_{n+1}) = (0.15, 0.4, 0.45)$ ,  $r^* = 2$

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

→ Ex 2:  $\hat{A}(\textcolor{violet}{X}_{n+1}) = (0.03, \textcolor{blue}{0.95}, 0.02)$ ,  $r^* = 1$

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

- **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)

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- **Marginal** theoretical guarantee over the joint  $(X, Y)$  distribution, and **not conditional**, i.e., no guarantee that for any  $x$ :

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

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

## Side comment: it is possible to achieve exactly $1 - \alpha$ coverage!

Note this other view on conformal sets, through conformal  $p$ -values:

$$\begin{aligned}\widehat{C}_\alpha(x) &= \left\{ y \in \mathcal{Y}, s(x, y; \hat{A}) \leq q_{1-\alpha}(\mathcal{S}) \right\} \\ &= \left\{ y \in \mathcal{Y}, \sum_{i \in \text{Cal}} \mathbb{1} \left\{ s(x, y; \hat{A}) > S_i \right\} < (1 - \alpha)(1 + \#\text{Cal}) \right\} \\ &= \left\{ y \in \mathcal{Y}, \frac{1 + \sum_{i \in \text{Cal}} \mathbb{1} \left\{ s(x, y; \hat{A}) \leq S_i \right\}}{1 + \#\text{Cal}} > \alpha \right\}.\end{aligned}$$

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The randomization procedures drawing  $U \sim \mathcal{U}([0, 1])$  and outputting:  $\widehat{C}_\alpha^r(x) :=$

$$\left\{ y \in \mathcal{Y}, \frac{\sum_{i \in \text{Cal}} \mathbb{1} \left\{ s(x, y; \hat{A}) < S_i \right\} + U \left( 1 + \sum_{i \in \text{Cal}} \mathbb{1} \left\{ s(x, y; \hat{A}) = S_i \right\} \right)}{\#\text{Cal} + 1} > \alpha \right\},$$

achieves **exactly  $1 - \alpha$  coverage** under exchangeability ([smoothed conformal prediction](#), Vovk et al., 2005).

Introductory remarks

Exchangeability

Split Conformal Prediction (SCP)

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

## SCP: what choices for the regression scores?

$$\widehat{C}_\alpha(\textcolor{violet}{X}_{n+1}) = \{y \text{ such that } \textcolor{blue}{s} \left( \textcolor{violet}{X}_{n+1}, y; \hat{\mathcal{A}} \right) \leq q_{1-\alpha}(\mathcal{S})\}$$

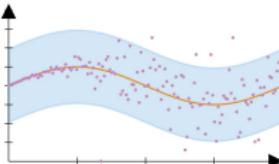
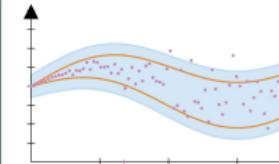
## SCP: what choices for the regression scores?

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

Standard SCP Vovk et al. (2005)			
$s(\hat{A}(X), Y)$	$ \hat{\mu}(X) - Y $		
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$		
Visu.			
✓	black-box around a “usable” prediction		
✗	not adaptive		

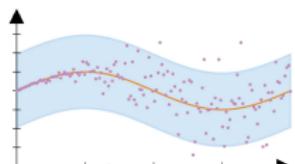
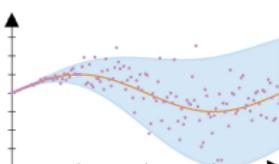
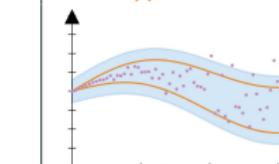
## SCP: what choices for the regression scores?

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

	Standard SCP Vovk et al. (2005)		CQR Romano et al. (2019)
$s(\hat{A}(X), Y)$	$ \hat{\mu}(X) - Y $		$\max(\widehat{QR}_{\text{lower}}(X) - Y,$ $Y - \widehat{QR}_{\text{upper}}(X))$ $[\widehat{QR}_{\text{lower}}(x) - q_{1-\alpha}(\mathcal{S});$ $\widehat{QR}_{\text{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$		
Visu.			
✓	black-box around a “usable” prediction		adaptive
✗	not adaptive		no black-box around a “usable” prediction

# SCP: what choices for the regression scores?

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

	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 $	$\frac{ \hat{\mu}(X) - Y }{\hat{\rho}(X)}$	$\max(\widehat{QR}_{\text{lower}}(X) - Y, Y - \widehat{QR}_{\text{upper}}(X))$ $[\widehat{QR}_{\text{lower}}(x) - q_{1-\alpha}(\mathcal{S})\hat{\rho}(x); \widehat{QR}_{\text{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)]$	
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

## Challenges that we are going to explore in the next lectures

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

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4. Beyond exchangeability (methods) (case studies)

## Challenges that we are going to explore in the next lectures

1. On exchangeability (theory)
2. Split conformal prediction (methods) (theory) (practical session)
3. Towards conditional coverage? (practical session) (theory) (case studies)
4. Beyond exchangeability (methods) (case studies)
5. Computational and statistical trade-offs (methods) (theory)
6. Handling missing data (methods)

## Some (other, non-exhaustives!) current open directions

- On conformal prediction efficiency (Bars and Humbert, 2025)
- Selective inference (Marandon et al., 2024a)
- Transductive conformal prediction, outlier detection (Vovk et al., 2003; Bates et al., 2023; Marandon et al., 2024b; Gazin et al., 2024)
- Aggregating predictive sets (Gasparin and Ramdas, 2024b,a; Gasparin et al., 2024)
- Multivariate outputs (Klein et al., 2025; Thurin et al., 2025; Kondratyev et al., 2025; Ndiaye, 2025)
- Beyond the indicator loss (Angelopoulos et al., 2022a; Bates et al., 2021; Angelopoulos et al., 2023; Lekeufack et al., 2024)
- Decision-theoretic foundations (Kiyani et al., 2025)

- CP is a very active field of research. Many developments focus on **adapting CP to specific frameworks**, such as:
  - Survival Analysis (Candès et al., 2023),
  - Causal Inference (Lei and Candès, 2021; Jin et al., 2023),
  - NLP (Schuster et al., 2022),
  - RL (Taufiq et al., 2022),
  - federated learning (Humbert et al., 2023; Plassier et al., 2023; Lu et al., 2023),
  - applications (medical (Angelopoulos et al., 2022b; Lu et al., 2022), energy (Kath and Ziel, 2021), etc.) and more.

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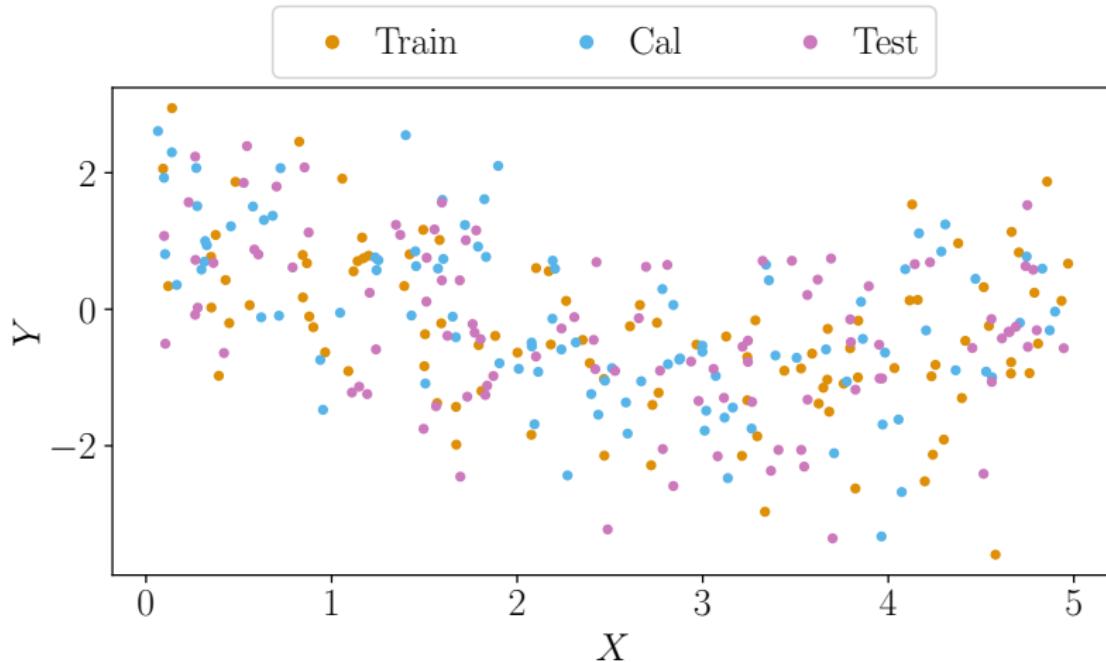
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SCP

CQR

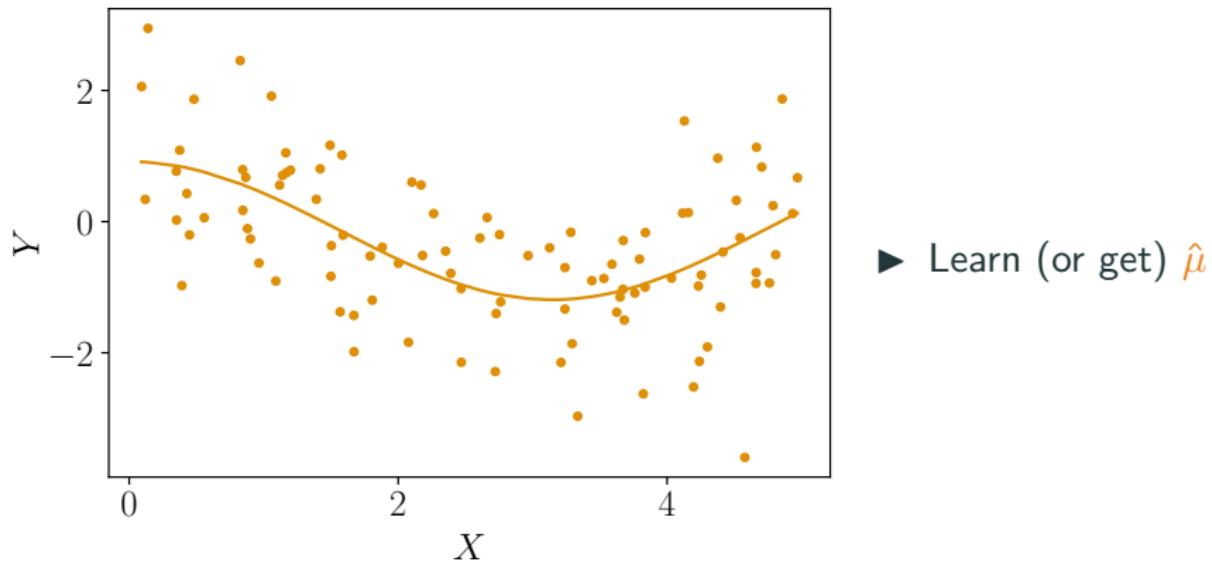
# Split Conformal Prediction (SCP)<sup>1,2,3</sup>: toy example



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

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

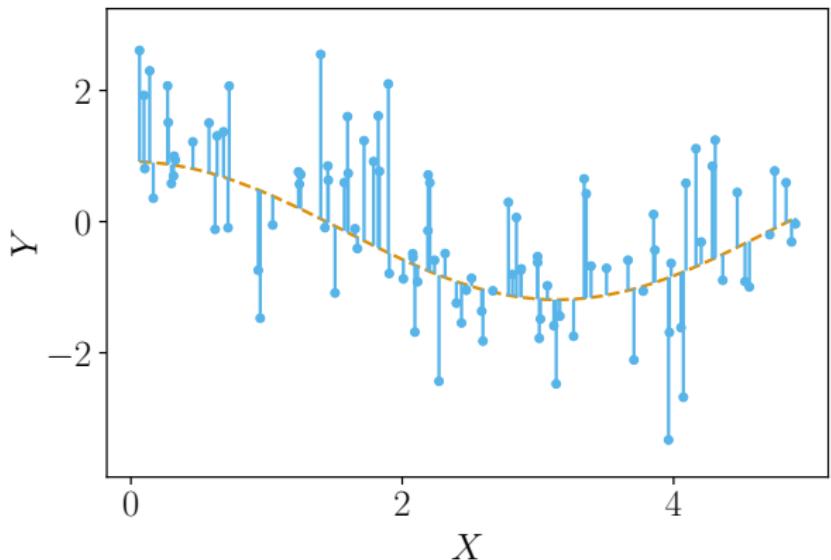
<sup>3</sup>Lei et al. (2018), *Distribution-Free Predictive Inference for Regression*, JRSS B



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

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

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



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

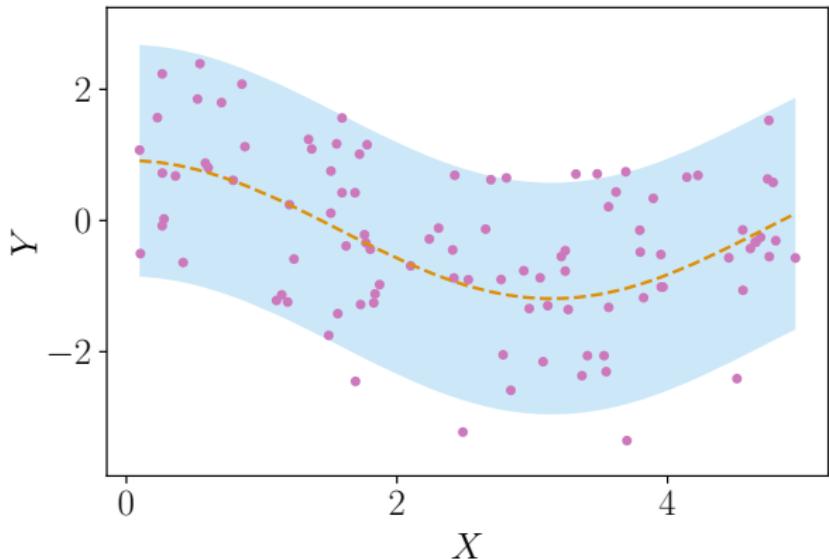
<sup>1</sup>Vovk et al. (2005), *Algorithmic Learning in a Random World*

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

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

# Split Conformal Prediction (SCP)<sup>1,2,3</sup>: toy example

prediction step



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

▶ Back to SCP

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

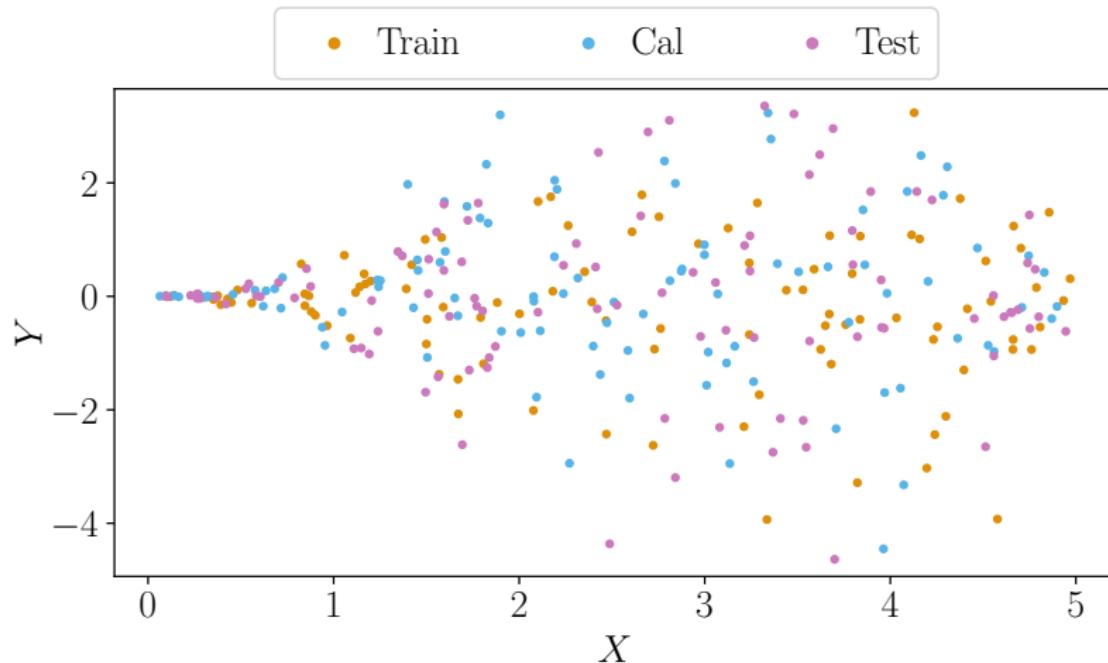
<sup>2</sup>Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML

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

SCP

CQR

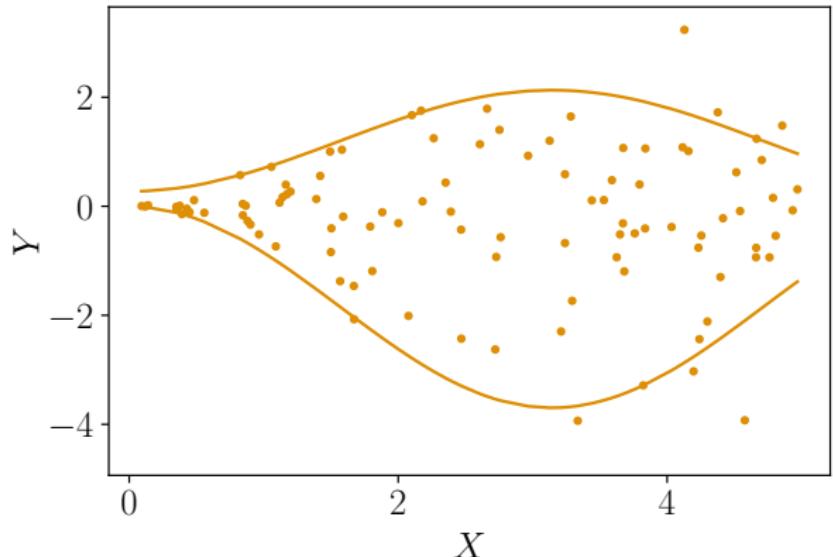
# Conformalized Quantile Regression (CQR)<sup>5</sup>



<sup>5</sup>Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

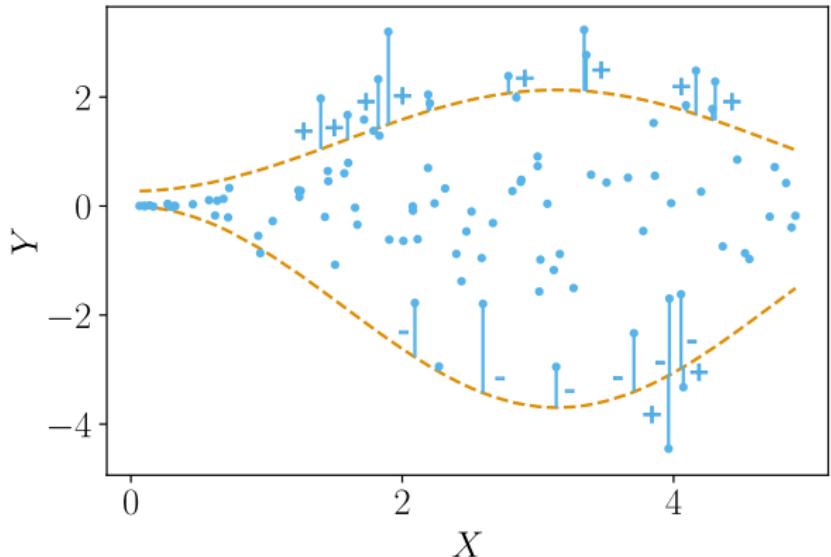
# Conformalized Quantile Regression (CQR)<sup>5</sup>

training step



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

<sup>5</sup>Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS



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

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

▶ Back to CQR

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<sup>5</sup>Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS