# Distribution-Free Uncertainty Quantification
# A short introduction to Conformal Prediction

Margaux Zaffran

## 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)

All material is freely accessible on this webpage, including sources.

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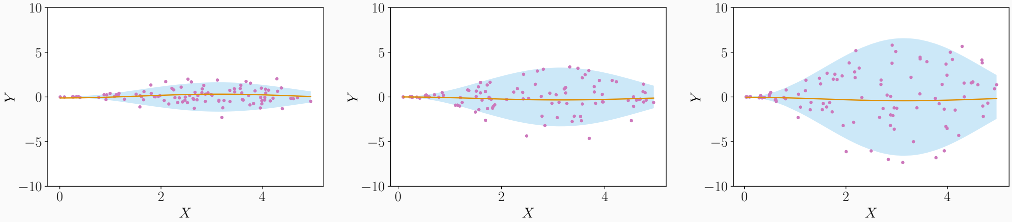
https://conformalpredictionintro.github.io

# On the importance of quantifying uncertainty




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

$\Longrightarrow$ Quantifying uncertainty conveys this information.

Quantile Regression

Split Conformal Prediction (SCP)

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

Beyond exchangeability

# 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 $q_\beta(X_1, \ldots, X_n)$
  $$:= \lceil \beta \times n \rceil \text{ smallest value of } (X_1, \ldots, X_n)$$

**Example of quantile: the median**

$\beta = 0.5$

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

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

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

# Median regression

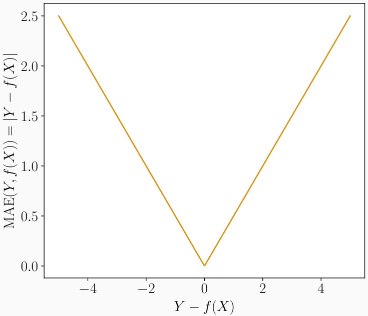
- The Bayes predictor depends on the chosen loss function.

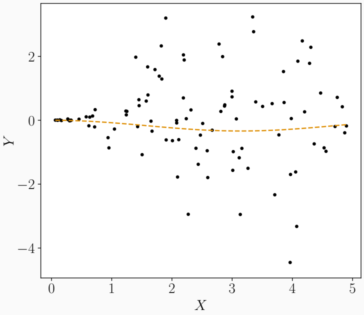
  $\hookrightarrow$ Bayes predictor $f^\star \in \underset{f}{\operatorname{argmin}} \operatorname{Risk}_\ell(f)$

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

- Mean Absolute Error (MAE): $\ell(Y, Y') = |Y - Y'|$ Associated risk: $\operatorname{Risk}_\ell(f) = \mathbb{E}\left[|Y - f(X)|\right]$

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



# Generalization: Quantile regression

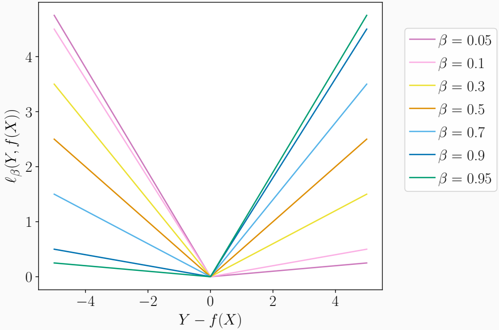
- Quantile level $\beta \in [0, 1]$
- Pinball loss

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

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

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

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

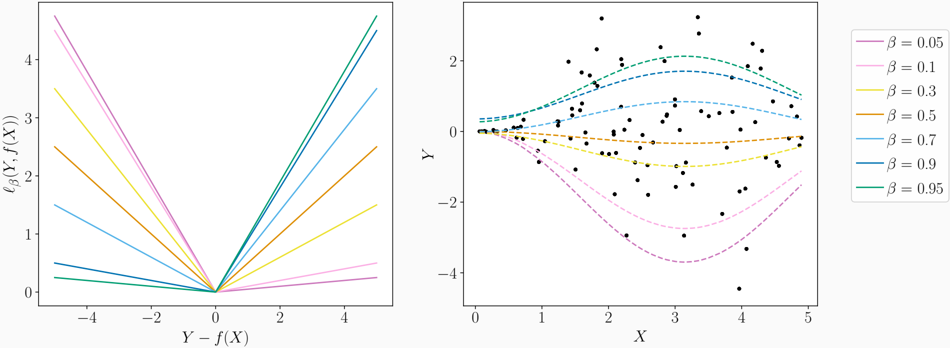


# Quantile regression: foundations

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

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

# Quantile regression: visualisation




**Warning**

No theoretical guarantee with a finite sample!

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

Quantile Regression

Split Conformal Prediction (SCP)

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

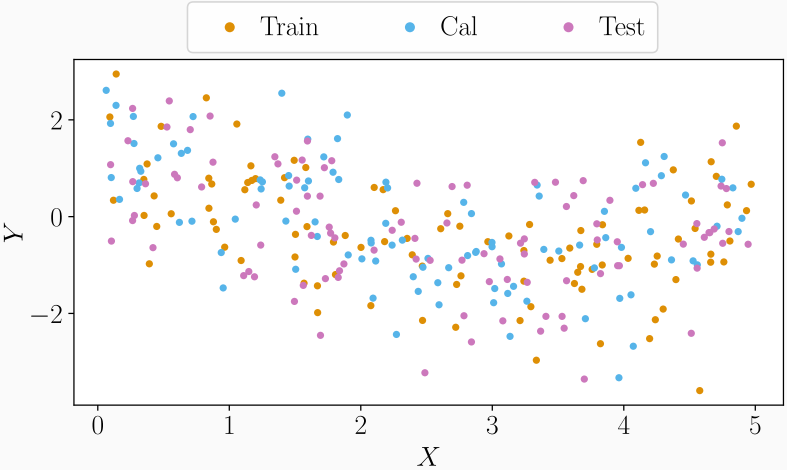
Avoiding data splitting: full conformal and out-of-bags approaches

Beyond exchangeability

# Quantifying predictive uncertainty

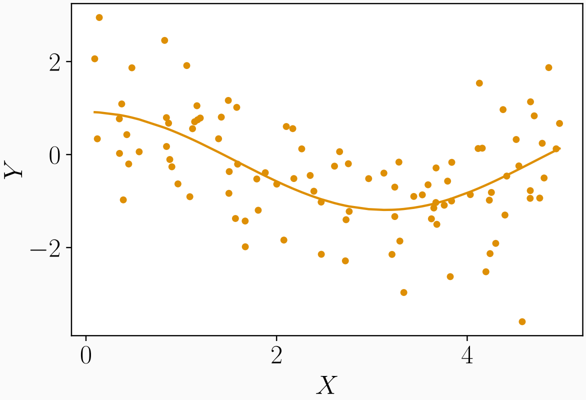
- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- $n$ training samples $(X_i, Y_i)_{i=1}^n$
- Goal: predict an unseen point $Y_{n+1}$ at $X_{n+1}$ with **confidence**
- How? Given a miscoverage level $\alpha \in [0, 1]$, build a predictive set $\mathcal{C}_\alpha$ such that:
$$\mathbb{P}\left\{Y_{n+1} \in \mathcal{C}_\alpha\left(X_{n+1}\right)\right\} \geq 1 - \alpha, \tag{1}$$
and $\mathcal{C}_\alpha$ should be as small as possible, in order to be informative
*For example:* $\alpha = 0.1$ and obtain a 90% coverage interval
- Construction of the predictive intervals should be
  - agnostic to the model
  - agnostic to the data distribution
  - valid in finite samples

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




[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*
[2] Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML
[3] Lei et al. (2018), *Distribution-Free Predictive Inference for Regression*, JRSS B

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




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

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

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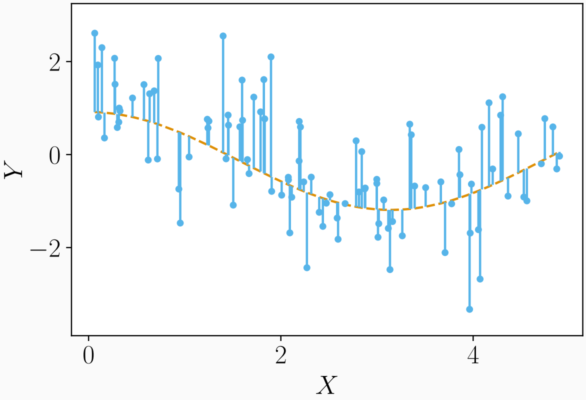
# Split Conformal Prediction (SCP)[1,2,3]: calibration step




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

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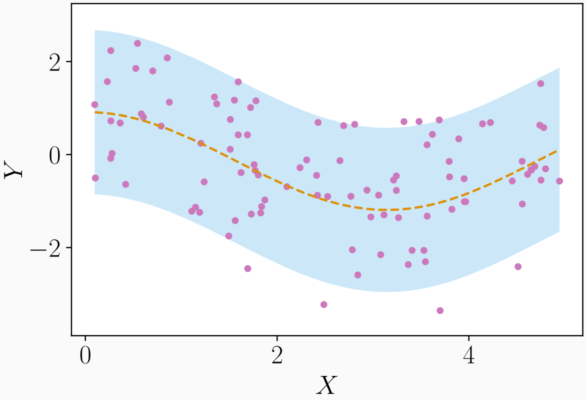
# Split Conformal Prediction (SCP)[1,2,3]: prediction step




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

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

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# SCP: implementation details


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

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

(+ worst-case scenario)

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

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

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

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

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# SCP: theoretical foundation

## Definition (Exchangeability)

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

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

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

## Examples of exchangeable sequences

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

## SCP: theoretical guarantees

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

**Theorem**

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

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

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

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

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

# Proof architecture of SCP guarantees

**Lemma (Quantile lemma)**

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

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

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

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

When $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable, the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ are exchangeable.
$\hookrightarrow$ applying the quantile lemma to the scores concludes the proof.

## Proof of the quantile lemma

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

Then, by definition of $q_\beta$:

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

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

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

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

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

$\square$

# SCP: theoretical guarantees

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

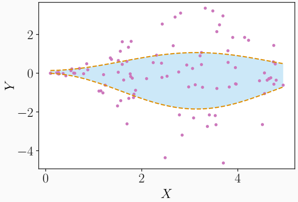
✗ Marginal coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) \cancel{| X_{n+1} = x}\right\} \geq 1 - \alpha$

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

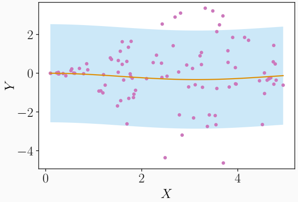
# Conditional coverage implies adaptiveness

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

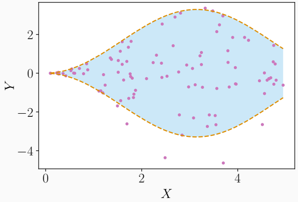
no coverage



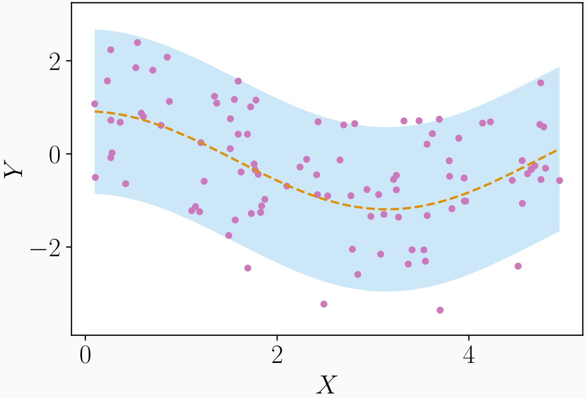

marginal




conditional



# Standard mean-regression SCP is not adaptive




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

# Informative conditional coverage as such is impossible

- Impossibility results

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

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

- Approximate conditional coverage

  $\hookrightarrow$ Romano et al. (2020a); Guan (2022); Jung et al. (2023); Gibbs et al. (2023)

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

- Asymptotic (with the sample size) conditional coverage

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

Non exhaustive references.

Quantile Regression

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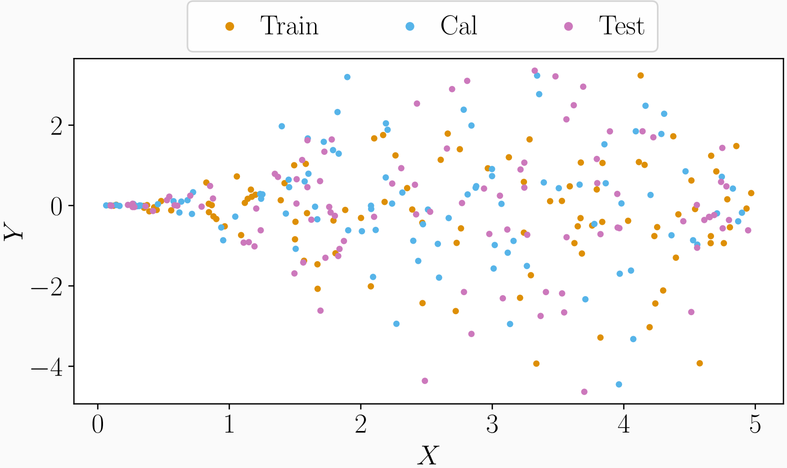
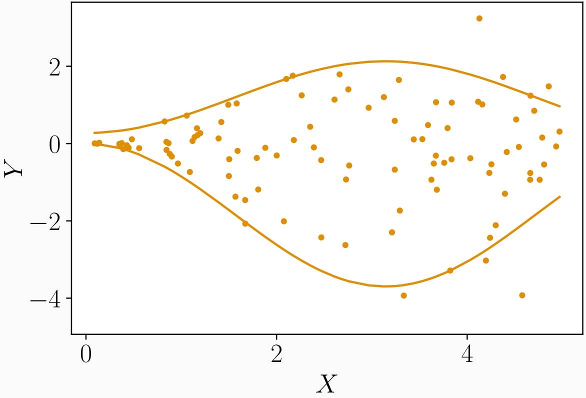
# Conformalized Quantile Regression (CQR)[5]




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

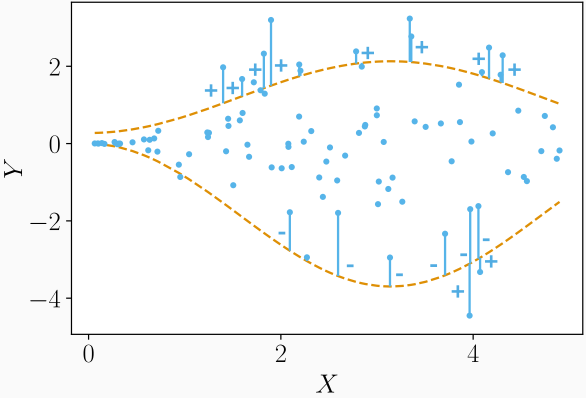
# Conformalized Quantile Regression (CQR)[5]: training step




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

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

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

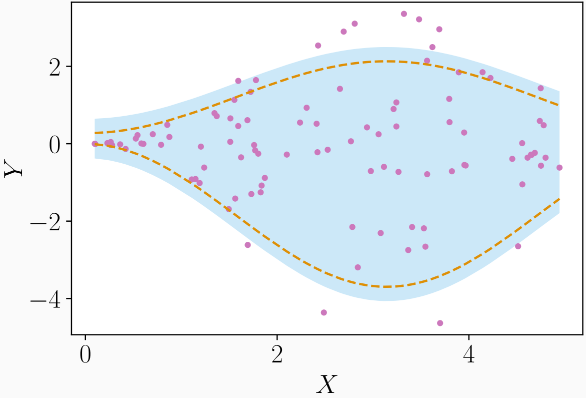



- Predict with $\widehat{\mathrm{QR}}_{\mathrm{lower}}$ and $\widehat{\mathrm{QR}}_{\mathrm{upper}}$
- Get the scores $\mathcal{S} = \{S_i\}_{\mathrm{Cal}} \cup \{+\infty\}$
- Compute the $(1-\alpha)$ empirical quantile of $\mathcal{S}$, noted $q_{1-\alpha}(\mathcal{S})$

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

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

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




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

- Build

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

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

# CQR: implementation details


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

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# CQR: theoretical guarantees

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

**Theorem**

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

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

*If, in addition, the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ are almost surely distinct, then*

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

Proof: application of the quantile lemma.

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

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

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# SCP is defined by the conformity score function


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

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

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

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

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

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

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

# SCP: theoretical guarantees

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

**Theorem**

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

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

*If, in addition, the scores* $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ *are almost surely distinct, then*

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

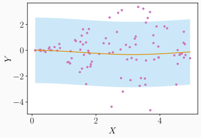
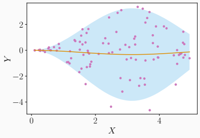
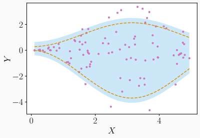
Proof: application of the quantile lemma.

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

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

# SCP: what choices for the regression scores?

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

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

# SCP: standard classification

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

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

# SCP: standard classification in practice

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

- Scores on the calibration set

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

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

# SCP: standard classification in practice, cont'd

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

- Scores on the calibration set

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

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

# SCP: limits of the standard classification case

The standard classification conformity score function leads to:

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

(similar to the standard mean regression case!)

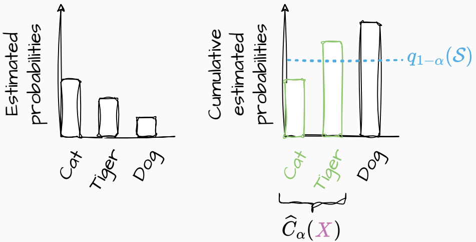
$\Rightarrow$ Other score functions can be built to improve adaptiveness

(as in regression with localized scores)

# SCP: classification with Adaptive Prediction Sets[8]

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

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




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

# SCP: classification with Adaptive Prediction Sets in practice

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

- Scores on the calibration set

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

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

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

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

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

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

# Split Conformal Prediction: summary

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

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

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

## Challenges: open questions (non exhaustive!)

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

Quantile Regression

Split Conformal Prediction (SCP)

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

- Full Conformal Prediction
- Jackknife+

Beyond exchangeability

# Splitting the data might not be desired

SCP suffers from data splitting:

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

Can we avoid splitting the data set?

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

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

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

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

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

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

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

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

# Full Conformal Prediction (CP): recovering exchangeability

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

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

✓ Test point treated in the same way than train points

✗ Computationally costly

# Full CP: theoretical foundation

**Definition (Symmetrical algorithm)**

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

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

# Full CP: theoretical guarantees

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

**Theorem**

*Suppose that*

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

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

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

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

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

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

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

**FCP sets with an interpolating algorithm**

Assume $\mathcal{A}$ interpolates:

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

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

Quantile Regression

Split Conformal Prediction (SCP)

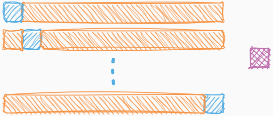
Avoiding data splitting: full conformal and out-of-bags approaches

Full Conformal Prediction

Jackknife+

Beyond exchangeability

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



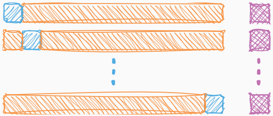
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO scores $\mathcal{S} = \left\{ |\hat{A}_{-i}(X_i) - Y_i| \right\}_i \cup \{+\infty\}$ (in standard mean regression)
- Get $\hat{A}$ by training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

**Warning**

No guarantee on the prediction of $\hat{A}$ with scores based on $(\hat{A}_{-i})_i$, without assuming a form of **stability** on $\mathcal{A}$.

# Jackknife+[10]

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



- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO predictions / predictive intervals

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

(in standard mean regression)

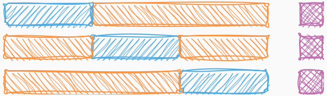
- Build the predictive interval: $[q_{\alpha,\inf}(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

**Theorem**

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

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

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



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

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

(in standard mean regression)

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

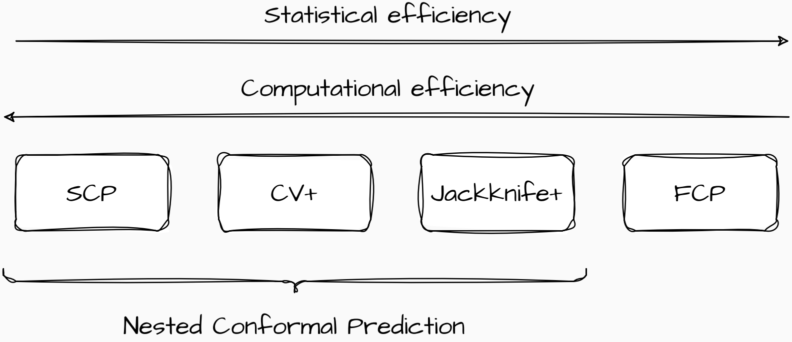
**Theorem**

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

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

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

# General overview




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

Non exhaustive references.

# Exchangeability does not hold in many practical applications

- CP requires exchangeable data points to ensure validity

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

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

✗ Arbitrary distribution shift

✗ Possibly many shifts, not only one

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

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

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

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

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

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

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

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

# Generalizations

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

# Online setting

- Data: $T_0$ random variables $(X_1, Y_1), \dots, (X_{T_0}, Y_{T_0})$ 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 $t \in [\![ T_0 + 1, T_0 + T_1 ]\!]$, $Y_{t-T_0}, \dots, Y_{t-1}$ have been revealed
- Build the smallest interval $\widehat{C}_\alpha^t$ such that:

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

often simplified in:

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

# Recent developments

- Consider splitting strategies that respect the temporal structure
- Gibbs and Candès (2021) propose a method which reacts faster to temporal evolution
  - Idea: track the previous coverages of the predictive intervals $(\mathbb{1}\{Y_t \in \widehat{C}_\alpha(X_t)\})$
  - Tool: update the empirical quantile level with a learning rate $\gamma$
  - Asymptotic guarantee (on average) for any distribution (even adversarial)
- Zaffran et al. (2022) studies the influence of this learning rate $\gamma$ and proposes, along with Gibbs and Candès (2022), a method not requiring to choose $\gamma$
- 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

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