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)

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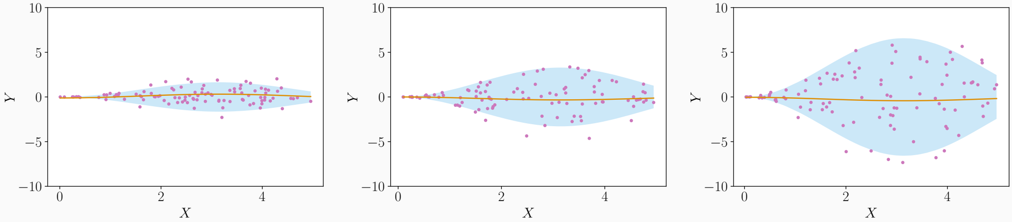
On the importance of quantifying uncertainty



↪ Same predictions, yet 3 distinct underlying phenomena!

⟹ 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 $q_\beta(X_1, \dots, X_n)$
  $:= \lceil \beta \times n \rceil$ smallest value of $(X_1, \dots, X_n)$

Example of quantile: the median

$\beta = 0.5$

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

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

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

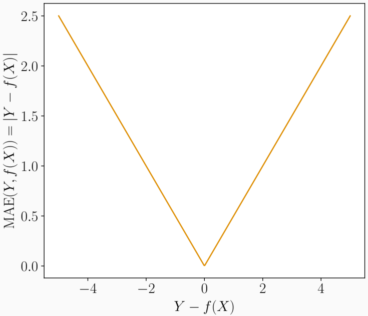
Median regression

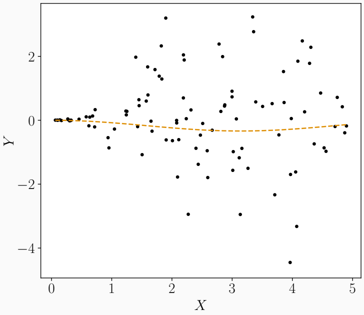
- The Bayes predictor depends on the chosen loss function.
  $\hookrightarrow$ Bayes predictor $f^\star \in \operatorname{argmin}_f \mathrm{Risk}_\ell(f)$

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

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

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





Generalization: Quantile regression

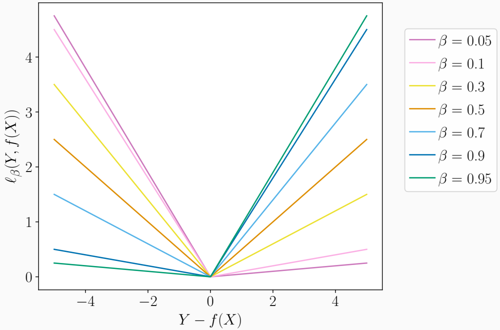
- Quantile level $\beta \in [0, 1]$
- Pinball loss

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

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

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

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

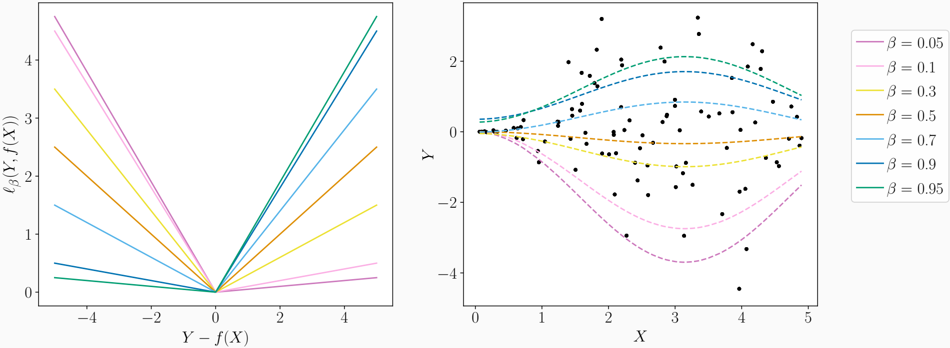


Quantile regression: foundations

- 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

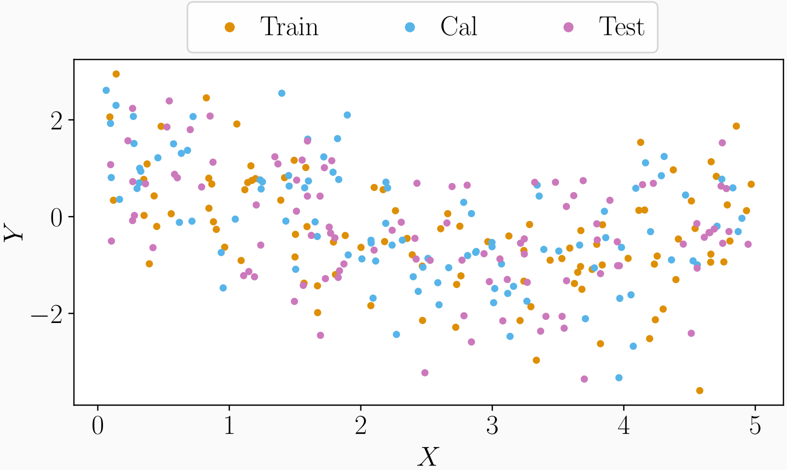
Avoiding data splitting: full conformal and out-of-bags approaches

Beyond exchangeability

Quantifying predictive uncertainty

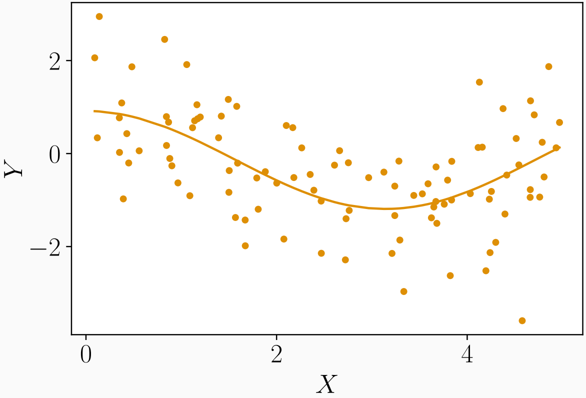
- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- n training samples $(X_i, Y_i)_{i=1}^n$
- Goal: predict an unseen point Y_{n+1} at X_{n+1} with **confidence**
- How? Given a miscoverage level $\alpha \in [0, 1]$, build a predictive set $\mathcal{C}_\alpha$ such that:
$$\mathbb{P}\left\{Y_{n+1} \in \mathcal{C}_\alpha\left(X_{n+1}\right)\right\} \geq 1 - \alpha, \tag{1}$$
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) $\hat{\mu}$

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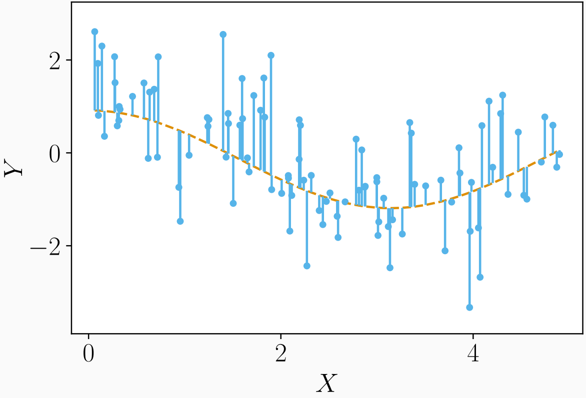
Split Conformal Prediction (SCP)[1,2,3]: calibration step



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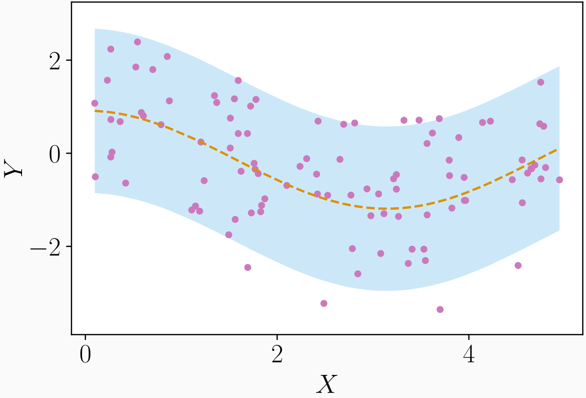
Split Conformal Prediction (SCP)[1,2,3]: prediction step



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

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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

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

SCP: implementation details

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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 $\#\mathrm{Cal}$ conformity scores:

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

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

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

SCP: theoretical foundation

Definition (Exchangeability)

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

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

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

Examples of exchangeable sequences

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

SCP: theoretical guarantees

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

Theorem

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

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

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.

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_β:

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

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

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

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

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

$\square$

SCP 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:*

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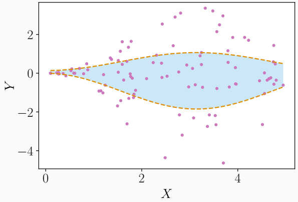
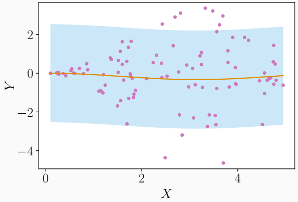
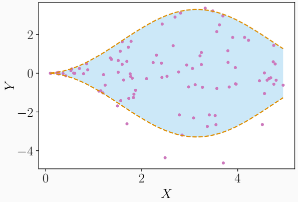
Additionally, if the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ *are a.s. distinct:*

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

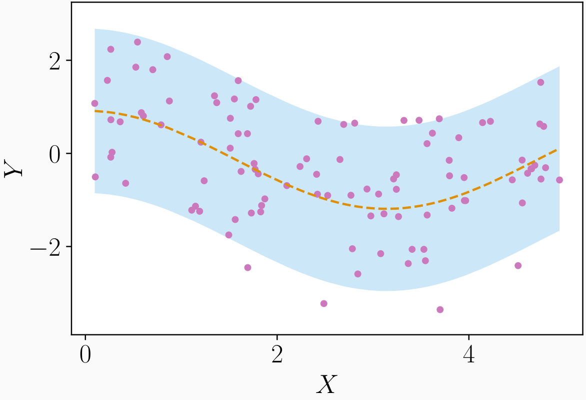
✗ Marginal coverage: $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) \cancel{| X_{n+1} = x}\right\} \geq 1 - \alpha$

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

- 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

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

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

- Approximate conditional coverage

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

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

- Asymptotic (with the sample size) conditional coverage

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

Non exhaustive references.

Quantile Regression

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- Standard regression case
- Conformalized Quantile Regression (CQR)
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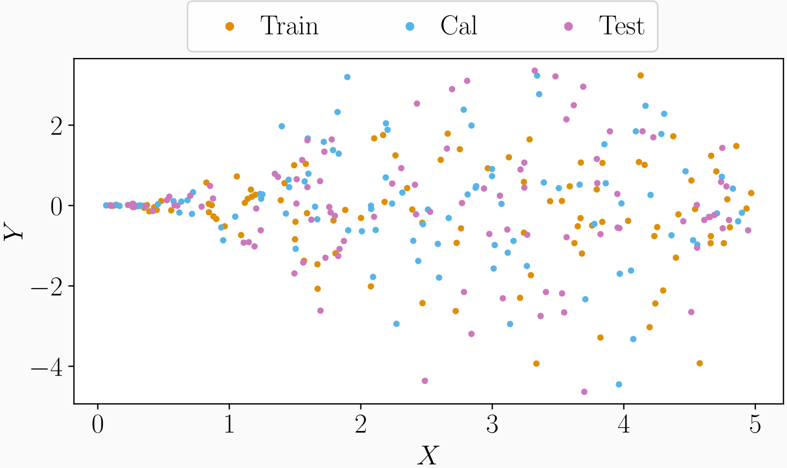
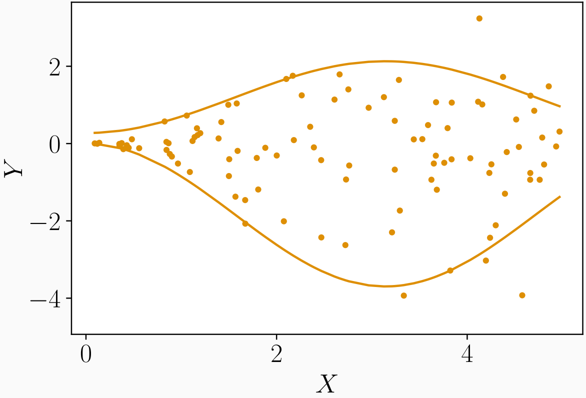
Beyond exchangeability

Conformalized Quantile Regression (CQR)[5]



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

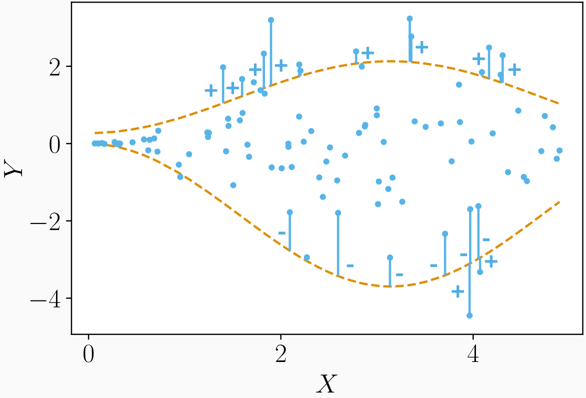
Conformalized Quantile Regression (CQR)[5]: training step



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

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

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

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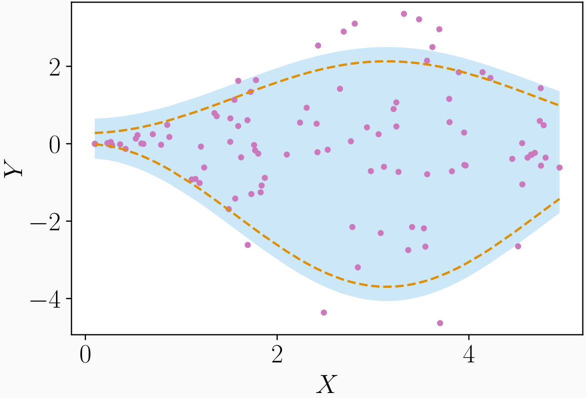
Conformalized Quantile Regression (CQR)[5]: prediction step



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

CQR: implementation details

1. Randomly split the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
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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.

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:

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

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

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

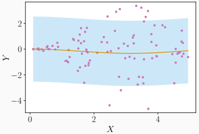
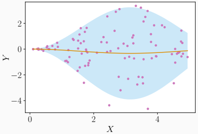
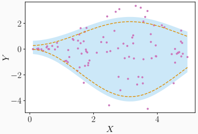
Proof: application of the quantile lemma.

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

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

SCP: what choices for the regression scores?

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

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

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

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

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

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

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

SCP: limits of the standard classification case

The standard classification conformity score function leads to:

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

(similar to the standard mean regression case!)

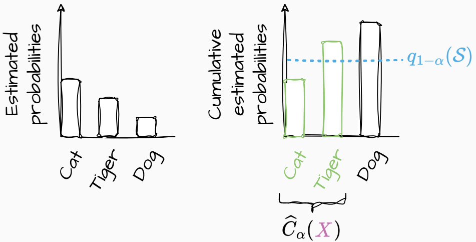
$\Rightarrow$ Other score functions can be built to improve adaptiveness

(as in regression with localized scores)

SCP: classification with Adaptive Prediction Sets[8]

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

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



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

SCP: classification with Adaptive Prediction Sets in practice

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

- Scores on the calibration set

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

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

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

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

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

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

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

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

$\hookrightarrow$ 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)

Splitting the data might not be desired

SCP suffers from data splitting:

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

Can we avoid splitting the data set?

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

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

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

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

✗ $\hat{A}$ has been obtained using the training set $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ but did not use X_{n+1}.
$\Rightarrow \mathrm{s}\left(\hat{A}(X_{n+1}), y\right)$ 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
$$\mathcal{S}_y^{(\text{train})} = \left\{ \mathrm{s}(\hat{A}_y(X_i), Y_i) \right\}_{i=1}^{n} \cup \{ \mathrm{s}(\hat{A}_y(X_{n+1}), y)\}$$
and compute their $1-\alpha$ empirical quantile $q_{1-\alpha}\left(\mathcal{S}_y^{(\text{train})}\right)$

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

✓ Test point treated in the same way than train points

✗ Computationally costly

Definition (Symmetrical algorithm)

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

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

Full CP: theoretical guarantees

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

Theorem

Suppose that

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

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

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

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

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

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

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

Interpolation regime

FCP sets with an interpolating algorithm

Assume $\mathcal{A}$ interpolates:

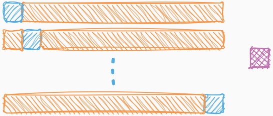
- $\hat{A} = \mathcal{A}\left((x_1, y_1), \dots, (x_{n+1}, y_{n+1})\right)$
- $\hat{A}(x_k) - y_k = 0$ for any $k \in [\![1, n+1]\!]$

$\Rightarrow$ 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

Jackknife: the naive idea does not enjoy valid coverage

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



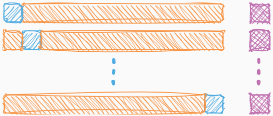
- $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO scores $\mathcal{S} = \left\{ |\hat{A}_{-i}(X_i) - Y_i| \right\}_i \cup \{+\infty\}$ (in standard mean regression)
- Get $\hat{A}$ by training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

Warning

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

Jackknife+[10]

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



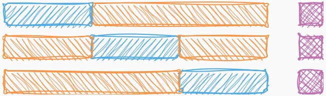
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
- Get $\hat{A}_{-i}$ by training $\mathcal{A}$ on $\mathcal{D}_n \setminus (X_i, Y_i)$
- LOO predictions / predictive intervals
  $$\mathcal{S}_{\text{up/down}} = \left\{ \hat{A}_{-i}(X_{n+1}) \pm |\hat{A}_{-i}(X_i) - Y_i| \right\}_i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

Theorem

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

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

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



- Based on cross-validation residuals
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ 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

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

(in standard mean regression)

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

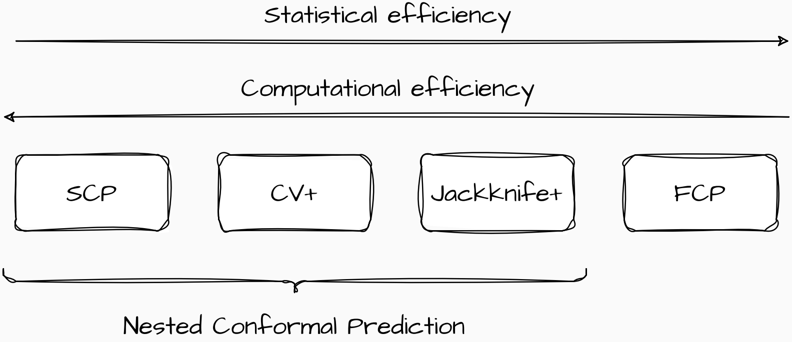
Theorem

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

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

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

Quantile Regression

Split Conformal Prediction (SCP)

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

Beyond exchangeability

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:
  - $(X_1, Y_1), \dots, (X_n, Y_n) \overset{i.i.d.}{\sim} P_X \times P_{Y|X}$
  - $(X_{n+1}, Y_{n+1}) \sim \tilde{P}_X \times P_{Y|X}$
- 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 $\widehat{C}_\alpha(X_{n+1}) =$
  $$\left\{ y : \boxed{\mathrm{s}}(\hat{A}(X_{n+1}), y) \leq q_{1-\alpha}\left(\{\omega_i^y S_i\}_{i \in \mathrm{Cal}} \cup \{+\infty\}\right) \right\}$$

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

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

often simplified in:

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

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 γ
  - Asymptotic guarantee (on average) for any distribution (even adversarial)
- Zaffran et al. (2022) studies the influence of this learning rate γ and proposes, along with Gibbs and Candès (2022), a method not requiring to choose γ
- Bhatnagar et al. (2023) enjoys **anytime** regret bound, by leveraging tools from the strongly adaptive regret minimization literature
- Bastani et al. (2022) proposes an algorithm achieving stronger coverage guarantees (conditional on specified overlapping subsets, and threshold calibrated) without hold-out set
- Angelopoulos et al. (2023) combines CP ideas with control theory ones, to adaptively improve the predictive intervals depending on the errors structure

Non exhaustive references.

References i

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. J., and Wasserman, L. (2018). Distribution-Free Predictive Inference for Regression. *Journal of the American Statistical Association*.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

https://conformalpredictionintro.github.io