

Predictive uncertainty quantification with missing covariates

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DATA Seminar

Inria



Who am I?

- 3rd (last) year statistics PhD Student, @ INRIA & École Polytechnique
- Funded by Électricité de France
- My advisors:



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Julie Josse

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- Research interests:
 - Distribution-free uncertainty quantification
 - Time series data
 - Missing values
 - Real life applications (energy, environmental, medical and societal domains)

Predictive Uncertainty Quantification with Missing Covariates



Yaniv Romano

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Conformal Prediction with Missing Values, ICML 2023

Predictive Uncertainty Quantification with Missing Covariates, submitted in 2024

(Way too short) Introduction to (Split) Conformal Prediction

Standard mean-regression case

Conformalized Quantile Regression (CQR)

Generalization of SCP: going beyond regression

Predictive Uncertainty Quantification with Missing Covariates

Final words

Quantifying predictive uncertainty

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- n training samples $(X^{(k)}, Y^{(k)})_{k=1}^n$
- **Goal:** predict an unseen point $Y^{(n+1)}$ at $X^{(n+1)}$ with **confidence**
- **How?** Given a miscoverage level $\alpha \in [0, 1]$, build a predictive set \mathcal{C}_α such that:

$$\mathbb{P} \left\{ Y^{(n+1)} \in \mathcal{C}_\alpha \left(X^{(n+1)} \right) \right\} \geq 1 - \alpha, \quad (1)$$

and \mathcal{C}_α should be as small as possible, in order to be informative.

For example: $\alpha = 0.1$ and obtain a 90% coverage interval

- ▶ Construction of the predictive intervals should be
 - agnostic to the model
 - agnostic to the data distribution
 - valid in finite samples

(Way too short) Introduction to (Split) Conformal Prediction

Standard mean-regression case

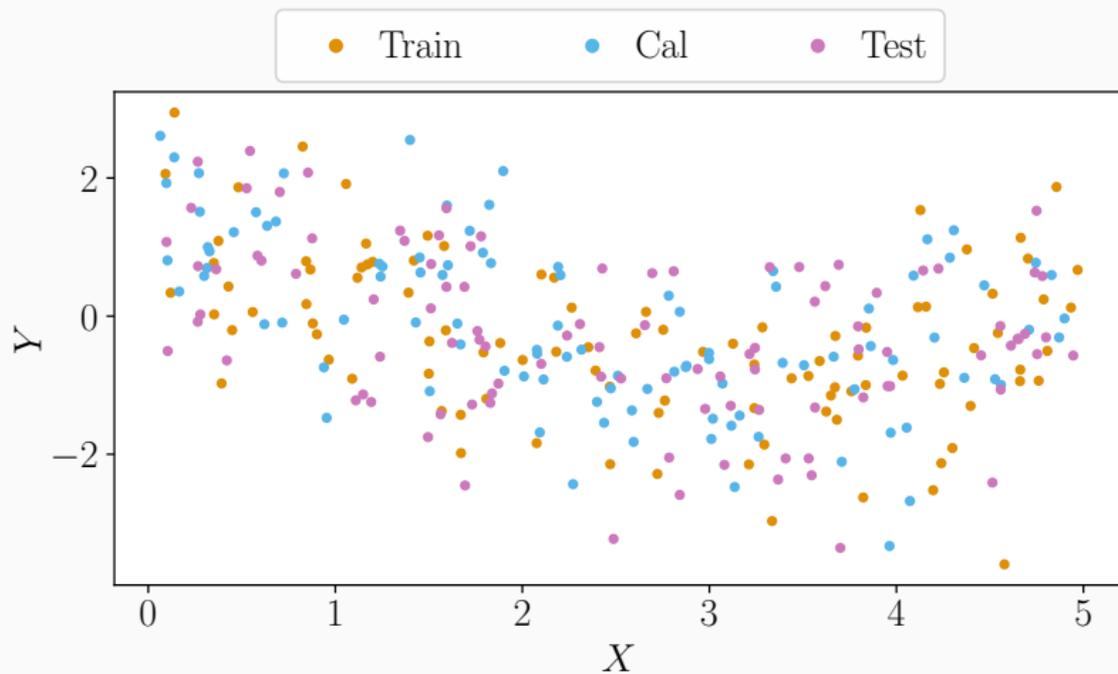
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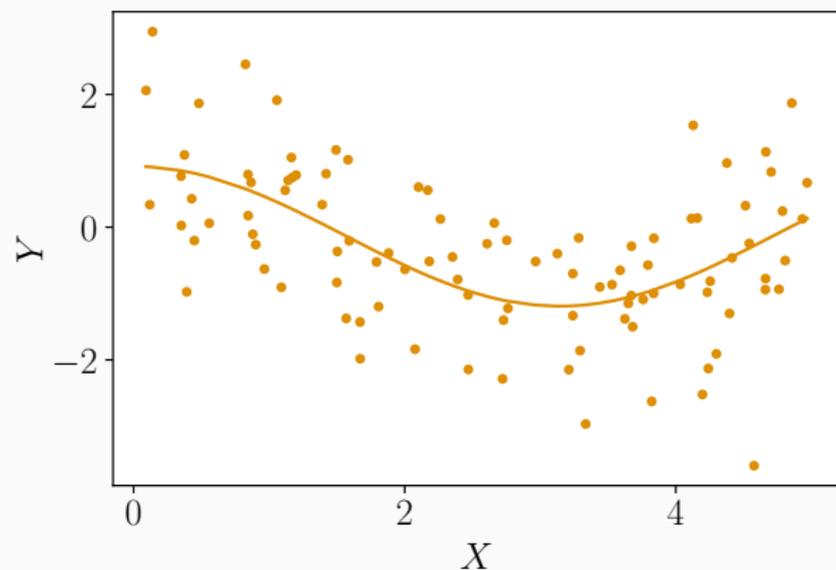
Split Conformal Prediction (SCP)^{1,2,3}: toy example



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

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

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

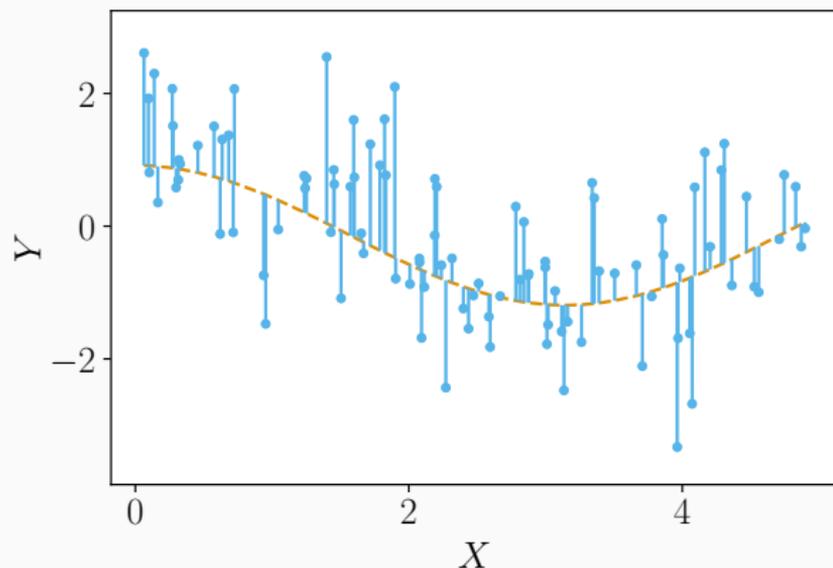


► Learn (or get) $\hat{\mu}$

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

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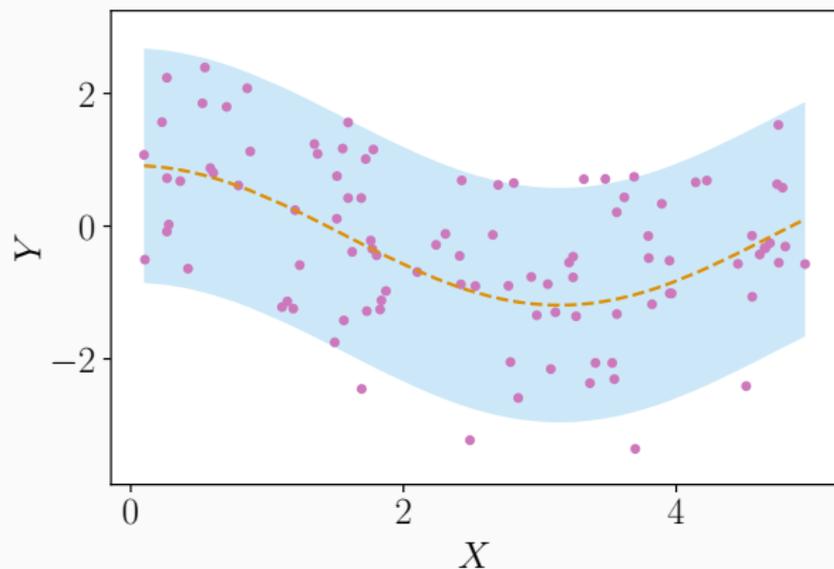


- ▶ Predict with $\hat{\mu}$
- ▶ Get the `|residuals|`, a.k.a. conformity scores
- ▶ Compute the $(1 - \alpha)$ empirical quantile of $\mathcal{S} = \{|\text{residuals}|\}_{\text{Cal}} \cup \{+\infty\}$, noted $q_{1-\alpha}(\mathcal{S})$

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

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

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



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

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

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Standard mean-regression SCP: implementation details

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

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

(+ worst-case scenario)

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

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

Exchangeability

$(X^{(k)}, Y^{(k)})_{k=1}^n$ are **exchangeable** if for any permutation σ of $\llbracket 1, n \rrbracket$ we have:

$$(X^{(1)}, Y^{(1)}), \dots, (X^{(n)}, Y^{(n)}) \stackrel{d}{=} (X^{(\sigma(1))}, Y^{(\sigma(1))}), \dots, (X^{(\sigma(n))}, Y^{(\sigma(n))}).$$

Examples of exchangeable sequences

- i.i.d. samples

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

Standard mean-regression SCP marginal validity (Vovk et al., 2005; Lei et al., 2018)

Suppose $(X^{(k)}, Y^{(k)})_{k=1}^{n+1}$ are **exchangeable (or i.i.d.)**^a. Standard mean-regression SCP applied on $(X^{(k)}, Y^{(k)})_{k=1}^n$ outputs $\widehat{C}_\alpha(\cdot)$ such that:

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

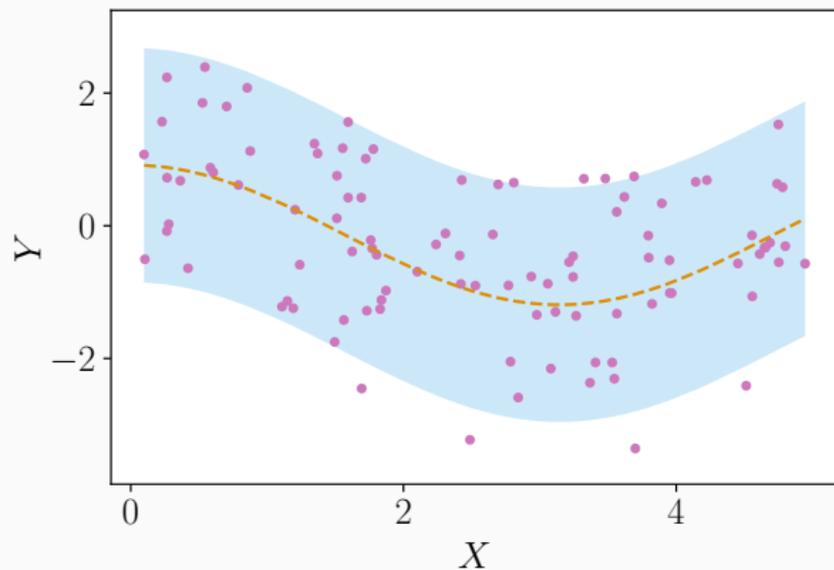
Additionally, if the scores $\{S^{(k)}\}_{k \in \text{Cal}} \cup \{S^{(n+1)}\}$ are a.s. distinct:

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

^aOnly the calibration and test data need to be exchangeable.

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

Standard mean-regression SCP is not adaptive



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

(Way too short) Introduction to (Split) Conformal Prediction

Standard mean-regression case

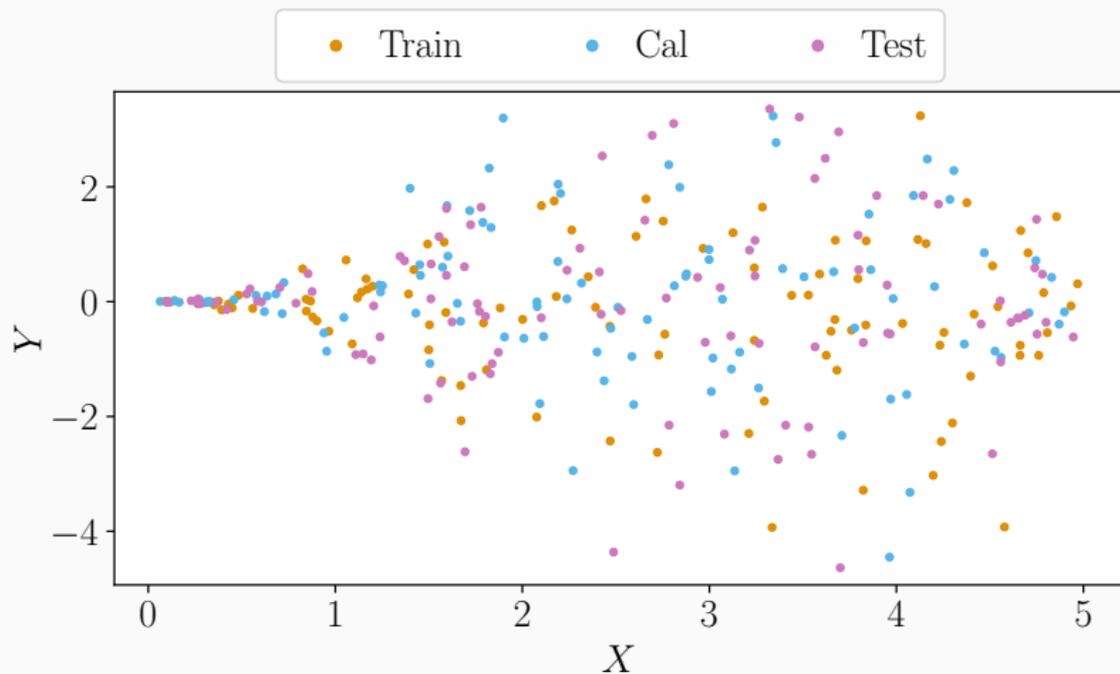
Conformalized Quantile Regression (CQR)

Generalization of SCP: going beyond regression

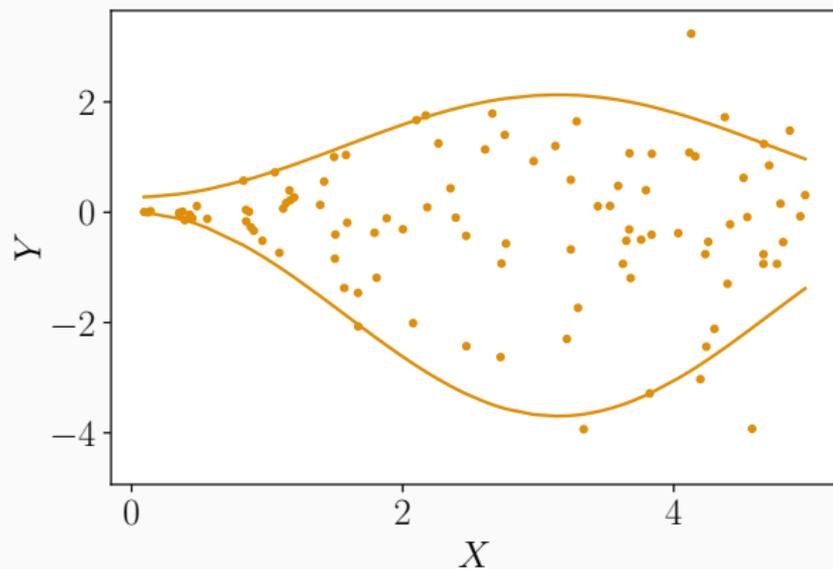
Predictive Uncertainty Quantification with Missing Covariates

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Conformalized Quantile Regression (CQR)⁴

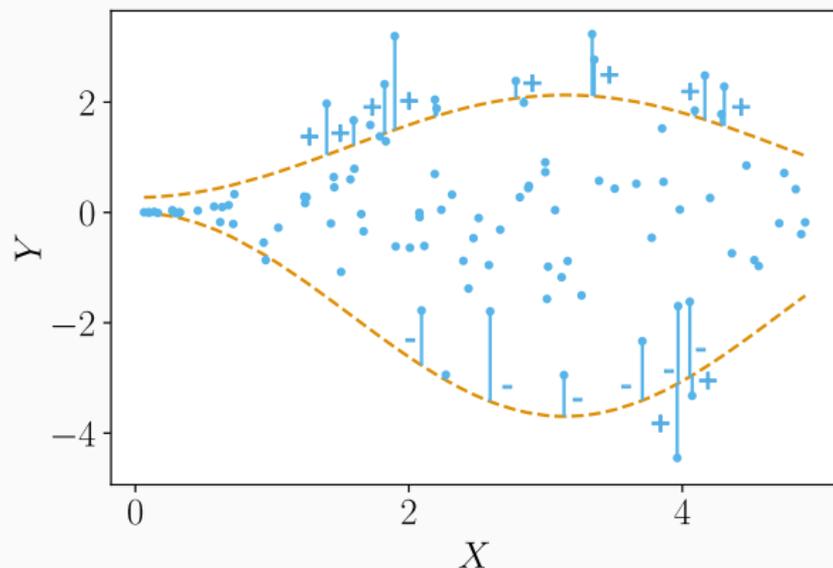


⁴Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS



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

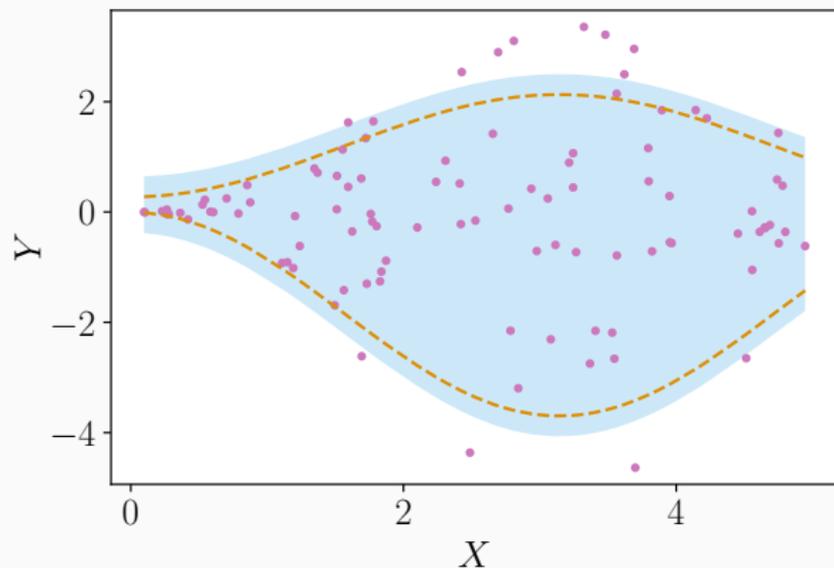
⁴Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS



- ▶ 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 $q_{1-\alpha}(\mathcal{S})$

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

⁴Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS



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

► Build

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

⁴Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

CQR marginal validity (Romano et al., 2019)

Suppose $(X^{(k)}, Y^{(k)})_{k=1}^{n+1}$ are **exchangeable (or i.i.d.)**^a. CQR applied on $(X^{(k)}, Y^{(k)})_{k=1}^n$ outputs $\hat{C}_\alpha(\cdot)$ such that:

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

Additionally, if the scores $\{S^{(k)}\}_{k \in \text{Cal}} \cup \{S^{(n+1)}\}$ are a.s. distinct:

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

^aOnly the calibration and test data need to be exchangeable.

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

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SCP is defined by the conformity score function

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

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

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

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

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

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

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

SCP marginal validity (Vovk et al., 2005)

Suppose $(X^{(k)}, Y^{(k)})_{k=1}^{n+1}$ are **exchangeable (or i.i.d.)**^a. SCP applied on $(X^{(k)}, Y^{(k)})_{k=1}^n$ outputs $\hat{C}_\alpha(\cdot)$ such that:

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

Additionally, if the scores $\{S^{(k)}\}_{k \in \text{Cal}} \cup \{S^{(n+1)}\}$ are a.s. distinct:

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

^aOnly the calibration and test data need to be exchangeable.

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

Split Conformal Prediction is simple to compute and works:

- ✓ any regression (and classification) algorithm (neural nets, random forest...);
- ✓ distribution-free as long as the data is exchangeable;
- ✓ finite sample.

✗ Note that the theoretical guarantee is **marginal** over the joint distribution of (X, Y) , and **not conditional**. In particular, **features conditional validity** is not ensured: there is no guarantee that for any $x \in \mathcal{X}$

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

Informative conditional coverage as such is impossible

- Impossibility results

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

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

- Approximate conditional coverage

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

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

- Asymptotic (with the sample size) conditional coverage

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

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Predictive Uncertainty Quantification with Missing Covariates

Supervised learning setting with missing values

Goals and challenges for predictive uncertainty quantification

Is MCV a too lofty goal?!

Achieving MCV under $M \perp\!\!\!\perp X$ and $Y \perp\!\!\!\perp M | X$

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Missing values are ubiquitous and challenging

Data: $(X^{(k)}, M^{(k)}, Y^{(k)})_{k=1}^n$

Y	X ₁	X ₂	X ₃	Mask M =		
				(M ₁	M ₂	M ₃)
22	5	6	3	0	0	0
19	6	8	NA	0	0	1
19	5	3	6	0	0	0
7	NA	9	NA	1	0	1
13	4	9	0	0	0	0
20	NA	NA	1	1	1	0
9	8	NA	4	0	1	0

↔ 2^d potential masks.

↔ M can depend on X or Y (depending on the missing mechanism⁵).

⇒ Statistical and computational challenges.

⁵Three mechanisms connecting X and M from Rubin (1976), *Inference and missing data*, Biometrika

Supervised learning with missing values: impute-then-regress

Impute-then-regress procedures are widely used.

1. Replace NA using an **imputation function** (e.g. the mean), noted ϕ .

$x^{(1)}$	-1	-10	6	0
$x^{(2)}$	4	NA	-2	2
$x^{(3)}$	5	1	2	NA
$x^{(4)}$	0	NA	NA	1

$\xrightarrow{\phi}$

$u^{(1)}$	-1	-10	6	0
$u^{(2)}$	4	-4.5	-2	2
$u^{(3)}$	5	1	2	1
$u^{(4)}$	0	-4.5	3	1

2. Train your algorithm (Random Forest, Neural Nets, etc.) on the **imputed**

$$\text{data: } \left\{ \underbrace{\phi \left(X_{\text{obs}(M^{(k)})}^{(k)}, M^{(k)} \right)}_{U^{(k)} = \text{imputed } X^{(k)}}, Y^{(k)} \right\}_{k=1}^n .$$

↪ we consider an **impute-then-regress** pipeline in this work.

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Goals of predictive uncertainty quantification with missing values

Goal: predict $Y^{(n+1)}$ with **confidence** $1 - \alpha$, i.e. build the smallest \mathcal{C}_α such that:

1. Marginal Validity (MV)

$$\mathbb{P} \left\{ Y^{(n+1)} \in \mathcal{C}_\alpha \left(X^{(n+1)}, M^{(n+1)} \right) \right\} \geq 1 - \alpha. \quad (\text{MV})$$

For example: $\alpha = 0.1$ and obtain a 90% coverage interval.

2. Mask-Conditional-Validity (MCV)

$$\mathbb{P} \left\{ Y^{(n+1)} \in \mathcal{C}_\alpha \left(X^{(n+1)}, m \right) \mid M^{(n+1)} \right\} \stackrel{\text{a.s.}}{\geq} 1 - \alpha. \quad (\text{MCV})$$

Exchangeability after imputation (Z., Dieuleveut, Josse and Romano, 2023)

Assume $(X^{(k)}, M^{(k)}, Y^{(k)})_{k=1}^n$ are i.i.d. (or exchangeable).

Then, for **any missing mechanism**, for almost **all imputation function**^a ϕ :
 $(\phi(X_{\text{obs}(M^{(k)})}^{(k)}, M^{(k)}), Y^{(k)})_{k=1}^n$ are **exchangeable**.

^aEven if the imputation is not accurate, the guarantee will hold.

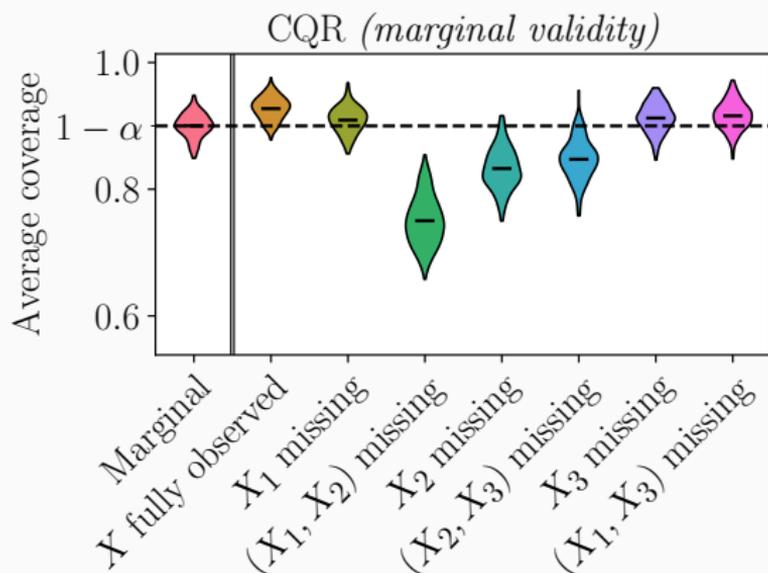
\Rightarrow CQR, and Conformal Prediction, applied on an imputed data set still enjoys marginal guarantees⁶:

$$\mathbb{P} \left\{ Y^{(n+1)} \in \widehat{C}_\alpha \left(X^{(n+1)}, M^{(n+1)} \right) \right\} \geq 1 - \alpha.$$

⁶The upper bound also holds under continuously distributed scores.

CQR is marginally valid on imputed data sets

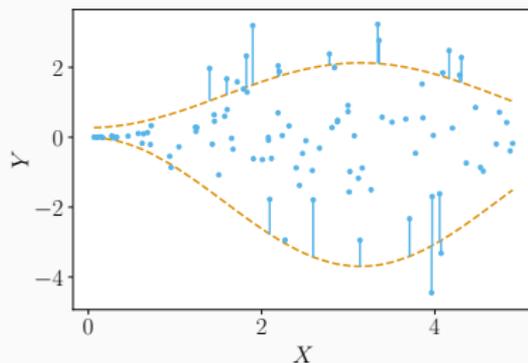
$$Y = \beta^T X + \varepsilon, \beta = (1, 2, -1)^T, X \text{ and } \varepsilon \text{ Gaussian.}$$



- ✓ Marginal (i.e. average) coverage (MV) is indeed recovered!
- ✗ Mask-conditional-validity (MCV) is not attained
 - ↪ Missing values induce heteroskedasticity
(supported by theory under (non-)parametric assumptions)

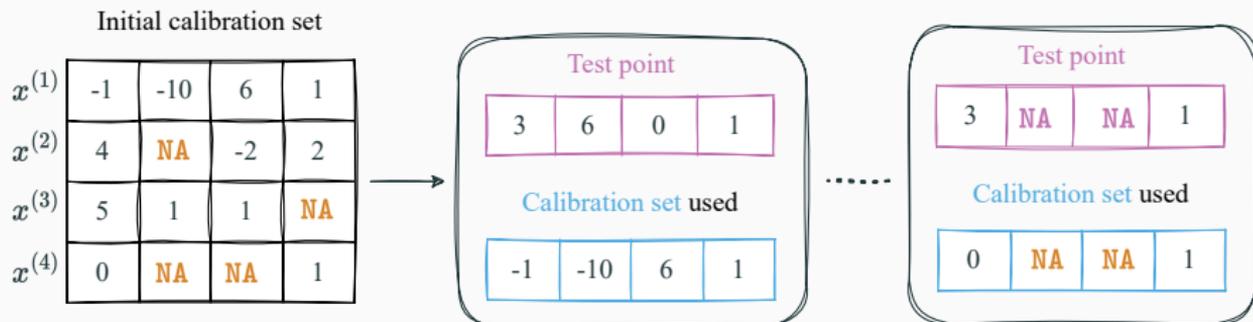
Conformalization step is independent of the important variable: the mask!

Observation: the α -correction term is computed among all the data points, regardless of their mask!



Warning: 2^d possible masks

⇒ Splitting the calibration set by mask is infeasible (lack of data)!



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General MCV hardness result (Z., Josse, Romano and Dieuleveut, 2024)⁷

If any \hat{C}_α is distribution-free MCV then **for any distribution** P , for any mask m such that $P_M(m) > 0$, it holds:

$$\mathbb{P}_{P^{\otimes(n+1)}} \left(\text{mes} \left(\hat{C}_\alpha (X_{n+1}, m) \right) = \infty \right) \geq 1 - \alpha - \Delta_{m,n} \geq 1 - \alpha - P_M(m)\sqrt{n+1}.$$

Irreducible term: consider \hat{C}_α outputting \mathcal{Y} with probability $1 - \alpha$ and \emptyset otherwise.

$\Delta_{m,n}$ term: smaller than $P_M(m)\sqrt{n+1}$

↪ gets negligible (making the lower bound nearly $1 - \alpha$) for low probability masks compared to n ;

↪ gets large (making the lower bound trivial because negative) for high probability masks compared to n .

⁷An analogous statement is also available for the classification framework.

Restricting the link between M and $(X \text{ or } Y)$ does not allow informative MCV

$M \perp\!\!\!\perp X$ hardness result (Z., Josse, Romano and Dieuleveut, 2024)

If any \widehat{C}_α is MCV under $M \perp\!\!\!\perp X$, then for any distribution P such that $M \perp\!\!\!\perp X$, for any mask m such that $P_M(m) > 0$, it holds:

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

$Y \perp\!\!\!\perp M \mid X$ hardness result (Z., Josse, Romano and Dieuleveut, 2024)

If any \widehat{C}_α is MCV under $Y \perp\!\!\!\perp M \mid X$, then for any distribution P such that $Y \perp\!\!\!\perp M \mid X$, for any mask m such that $\frac{1}{\sqrt{2}} \geq P_M(m) > 0$, it holds:

$$\mathbb{P}_{P^{\otimes(n+1)}} \left(\text{mes} \left(\widehat{C}_\alpha (X_{n+1}, m) \right) = \infty \right) \geq 1 - \alpha - \Delta_{m,n} \geq 1 - \alpha - 2P_M(m) \sqrt{n+1}.$$

\Rightarrow need to restrict both the link between M and X , as well as between M and Y .

Analogous statements are also available for the classification framework.

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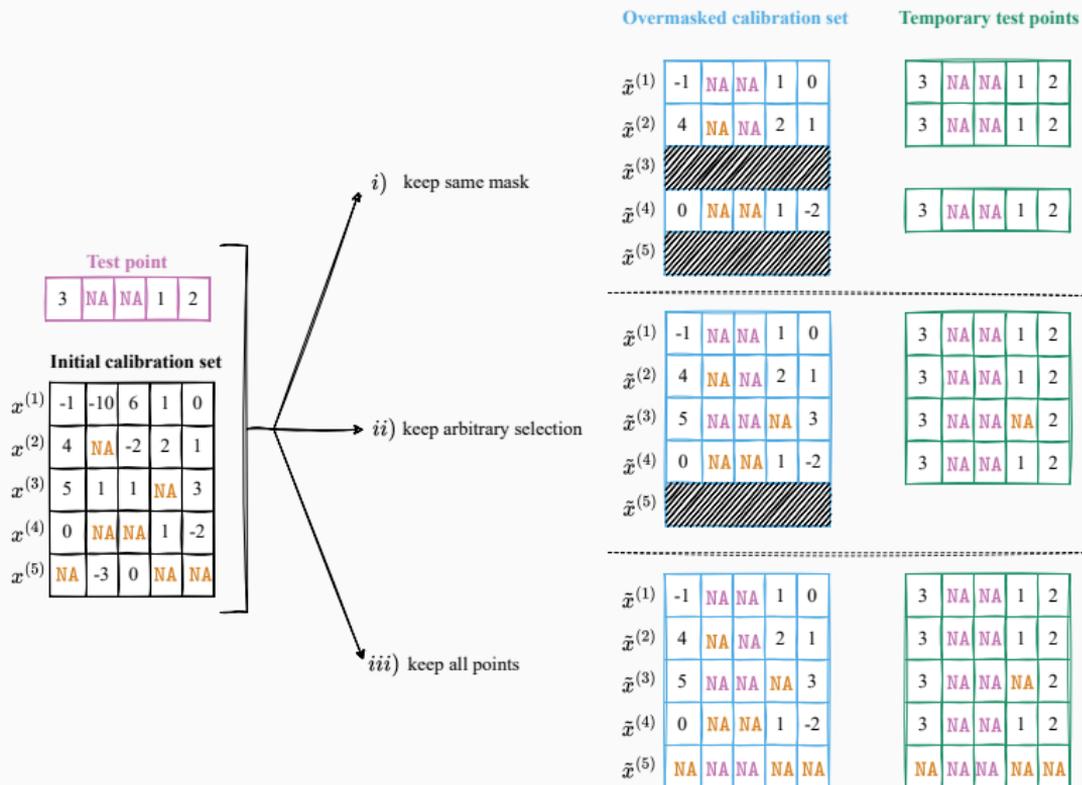
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Idea: for each **test point**, modify the **calibration points** to mimic the **test mask**



Mask-conditional-validity of CP-MDA-Nested*
(Z., Josse, Romano and Dieuleveut, 2024)

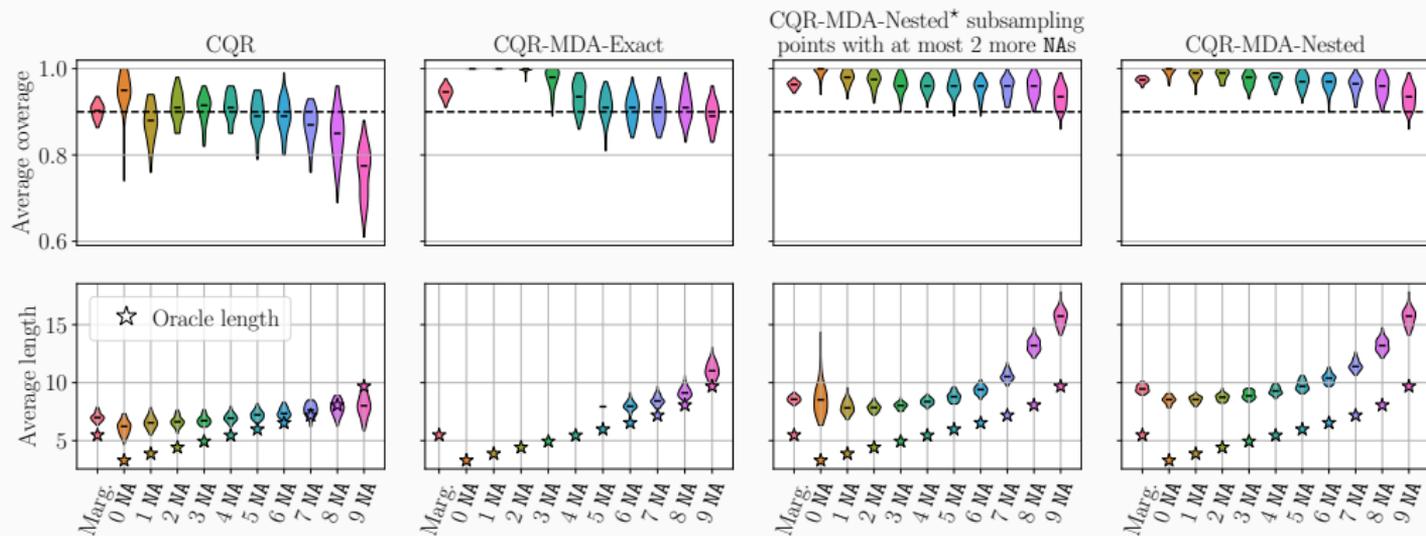
Under the assumptions that:

- $M \perp\!\!\!\perp X$,
- $Y \perp\!\!\!\perp M \mid X$,
- $(X^{(k)}, M^{(k)}, Y^{(k)})_{k=1}^{n+1}$ are i.i.d.,
- the subsampling scheme is independent of $(X^{(k)}, Y^{(k)})_{k=1}^{n+1}$,

then, for almost all imputation function, CP-MDA-Nested* reaches (MCV) at the level $1 - 2\alpha$, that is:

$$\mathbb{P} \left\{ Y^{(n+1)} \in \widehat{C}_\alpha \left(X^{(n+1)}, m \right) \mid M^{(n+1)} \right\} \stackrel{a.s.}{\geq} 1 - 2\alpha.$$

Experiments on $M \perp X$ and $Y \perp M | X$ Gaussian linear data in dimension 10



40% of missing values

- Under various MAR and MNAR mechanisms, CP-MDA-Nested* maintains empirical MCV;
- When $Y \not\perp M | X$ and the imputation is not accurate enough, CP-MDA-Nested* fails to empirically ensure MCV, with a loss of coverage that is more critical when subsampling.

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Predictive Uncertainty Quantification with Missing Covariates

Final words

- CP marginal guarantees hold on the imputed data set.
- CQR (and more generally CP) fails to attain coverage conditional on the missing pattern, i.e. MCV.
- Missingness introduces additional heteroskedasticity.
- MCV is impossible to ensure in an informative way without restricting both the dependence between M and X , and between M and Y .
- CP-MDA-Nested* (Missing Data Augmentation) is the first method to output predictive intervals with missing values.
- CP-MDA-Nested* attains conditional coverage with respect to the missing pattern (in MCAR and $Y \perp\!\!\!\perp M \mid X$ setting).
- CP-MDA-Nested* is empirically robust to non-MCAR scenarii.

- Consistency of universal quantile learner when chained with almost any imputation function (Z., Dieuleveut, Josse and Romano, 2023)
- (Non-)Parametric modelizations of the missing covariates' influence on predictive uncertainty (Z., Josse, Romano and Dieuleveut, 2024)
- Other theoretical guarantees on CP-MDA-Nested* (Z., Dieuleveut, Josse and Romano, 2023; Z., Josse, Romano and Dieuleveut, 2024)
- Critical care medical data experiments (Z., Dieuleveut, Josse and Romano, 2023)

A natural open direction: is it possible to achieve MCV under MAR and $Y \perp M | X$ assumptions?

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