# **Conformal Prediction with Missing Values**

Margaux Zaffran Stats Workshop (FAST-BIG)





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Conformal Prediction with Missing Values

# Setting

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$  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  $\mathcal{C}_{\alpha}$  such that:

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

and  $C_{\alpha}$  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

# (Way too short) Intro to (Split) Conformal Prediction Standard Split Conformal Prediction for Mean-Regression Improving Adaptiveness: Conformalized Quantile Regression

Conformal Prediction with Missing Values

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



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



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

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Predict with \$\hu\$
Build \$\hu\$
\$\hu\$<

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# **Definition (Exchangeability)**

 $(X^{(k)}, Y^{(k)})_{k=1}^{n}$  are exchangeable if for any permutation  $\sigma$  of [[1, n]] we have:

$$\mathcal{L}\left(\left(X^{(1)}, Y^{(1)}\right), \dots, \left(X^{(n)}, Y^{(n)}\right)\right) \\ = \mathcal{L}\left(\left(X^{(\sigma(1))}, Y^{(\sigma(1))}\right), \dots, \left(X^{(\sigma(n))}, Y^{(\sigma(n))}\right)\right)$$

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

### Examples of exchangeable sequences

- i.i.d. samples
- ${\mbox{ \bullet}}$  The components of  ${\mathcal N}$

$$\begin{pmatrix} m \\ \vdots \\ \vdots \\ m \end{pmatrix}, \begin{pmatrix} \sigma^2 & & \\ & \ddots & \gamma^2 & \\ & \gamma^2 & \ddots & \\ & & & & \sigma^2 \end{pmatrix} \end{pmatrix}$$

# SCP: theoretical guarantees

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

#### Theorem

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

$$\mathbb{P}\left\{Y^{(n+1)} \in \widehat{C}_{\alpha}\left(X^{(n+1)}\right)\right\} \ge 1 - \alpha.$$
Additionally, if the scores  $\{S^{(k)}\}_{k\in \operatorname{Cal}} \cup \{S_{n+1}\}$  are a.s. distinct:  

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

- Distribution-free, only requires exchangeability
- Any regression algorithm (neural nets, random forest...)
- Finite sample

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

### (Way too short) Intro to (Split) Conformal Prediction

Standard Split Conformal Prediction for Mean-Regression

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

# Conformalized Quantile Regression (CQR)<sup>4</sup>



<sup>&</sup>lt;sup>4</sup>Romano et al. (2019), Conformalized Quantile Regression, NeurIPS



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<sup>&</sup>lt;sup>4</sup>Romano et al. (2019), *Conformalized Quantile Regression*, NeurIPS

CQR enjoys finite sample guarantees proved in Romano et al. (2019), as a particular case of Split Conformal Prediction (SCP).

#### Theorem

$$\begin{split} & \text{Suppose } \left(X^{(k)}, Y^{(k)}\right)_{k=1}^{n+1} \text{ are exchangeable (or i.i.d.). CQR applied on} \\ & \left(X^{(k)}, Y^{(k)}\right)_{k=1}^{n} \text{ outputs } \widehat{C}_{\alpha}\left(\cdot\right) \text{ such that:} \\ & \mathbb{P}\left\{Y^{(n+1)} \in \widehat{C}_{\alpha}\left(X^{(n+1)}\right)\right\} \geq 1 - \alpha. \\ & \text{Additionally, if the scores } \left\{S^{(k)}\right\}_{k \in \operatorname{Cal}} \cup \left\{S_{n+1}\right\} \text{ are a.s. distinct:} \\ & \mathbb{P}\left\{Y^{(n+1)} \in \widehat{C}_{\alpha}\left(X^{(n+1)}\right)\right\} \leq 1 - \alpha + \frac{1}{\#\operatorname{Cal} + 1}. \end{split}$$

- Distribution-free, only requires exchangeability
- Any quantile regression algorithm (neural nets, random forest...)
- Finite sample

× Marginal coverage:  $\mathbb{P}\left\{Y^{(n+1)} \in \widehat{C}_{\alpha}\left(X^{(n+1)}\right) | X^{(n+1)} = x\right\} \ge 1 - \alpha$  conditional 7/17

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

Conformal Prediction with Missing Values

# Missing values are ubiquitous and challenging

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

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Y	$X_1$	$X_2$	$X_3$	$(M_1$	$M_2$	$M_3)$
22.42	0.55	0.67	0.03	0	0	0
8.26	0.72	0.18	0.55	0	0	0
19.41	0.60	0.58	NA	0	0	1
19.75	0.54	0.43	0.96	0	0	0
7.32	NA	0.19	NA	1	0	1
13.55	0.65	0.69	0.50	0	0	0
20.75	NA	NA	0.61	1	1	0
9.26	0.89	NA	0.84	0	1	0
9.68	0.963	0.45	0.65	0	0	0

# $\hookrightarrow 2^d$ potential masks.

- $\hookrightarrow M$  can depend on X or Y (depending on the missing mechanism).
- $\Rightarrow$  Statistical and computational challenges.

Impute-then-regress procedures are widely used.

1. Replace NA using an imputation function (e.g. the mean), noted  $\phi$ .



2. Train your algorithm (Random Forest, Neural Nets, etc.) on the imputed data:  $\left\{ \begin{array}{c} \phi(X^{(k)}, M^{(k)}), Y^{(k)} \\ \downarrow^{(k) = \text{imputed } X^{(k)}} \end{array} \right\}_{k=1}^{n}.$ 

 $\hookrightarrow$  we consider an impute-then-regress pipeline in this work.

### Predictive uncertainty quantification with missing values

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

1. Marginal Validity (MV)

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

2. Mask-Conditional-Validity (MCV)

$$\forall m \in \{0,1\}^d : \mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_{\alpha}\left(X^{(n+1)}, m\right) | M^{(n+1)} = m\right\} \ge 1 - \alpha. \quad (\mathsf{MCV})$$



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# CP is marginally valid (MV) after imputation

To apply conformal prediction we need exchangeable data.

#### Lemma

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<sup>5</sup>  $\phi$ :  $(\phi(X^{(k)}, M^{(k)}), Y^{(k)})_{k=1}^{n}$  are exchangeable.

 $\Rightarrow$  CQR, and Conformal Prediction, applied on an imputed data set still enjoys marginal guarantees<sup>6</sup>:

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

<sup>&</sup>lt;sup>5</sup>Even if the imputation is not accurate, the guarantee will hold.

<sup>&</sup>lt;sup>6</sup>The upper bound also holds under continuously distributed scores.

# CQR is marginally valid on imputed data sets

$$Y=eta^{ op}X+arepsilon,\ eta=(1,2,-1)^{ op},\ X$$
 and  $arepsilon$  Gaussian.



• The predictive uncertainty strongly depends on the mask

	$Imputation{+}CQR$	
(MV)	$\checkmark$	
(MCV)	×	

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

**Observation:** the  $\alpha$ -correction term is computed  $\succ$  among all the data points, regardless of their mask!



# **Warning:** $2^d$ possible masks

 $\Rightarrow$  Splitting the calibration set by mask is infeasible (lack of data)!



# Missing Data Augmentation (MDA)

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

Test point



Algorithms: MDA with Exact masking or with Nested masking.



### Theorem (Informal)

If  $M \perp (X, Y)$ , for almost all imputation function, CP-MDA reaches (MCV).



	$Imputation{+}CQR$	CQR-MDA
(MV)	$\checkmark$	✓
(MCV)	×	$\checkmark$

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- CP marginal guarantees hold on the imputed data set.
- Missingness introduces additional heteroskedasticity, creating a need for quantile regression based methods.
- CQR fails to attain coverage conditional on the missing pattern.
- Missing data augmentation is the first method to output predictive intervals with missing values.
- Missing data augmentation attains conditional coverage with respect to the missing pattern (in MCAR setting).
- Extensions:
  - Synthetic experiments in higher dimension
  - Semi-synthetic experiments
  - $\circ~$  Synthetic experiments beyond MCAR (MAR and MNAR)
  - Real data experiments (TraumaBase)
  - CP-MDA-Nested (link to CP-MDA-Nested), an algorithm which does not discard any calibration point
  - $\circ$  Consistency of universal quantile learner when chained with almost any

# Questions? :)

# Thanks for listening and feel free to reach out!



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# Informative conditional coverage as such is impossible

• Impossibility results

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

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

• Approximate conditional coverage

 $\hookrightarrow$  Romano et al. (2020); Guan (2022); Jung et al. (2023); Gibbs et al. (2023) Target  $\mathbb{P}(Y_{n+1} \in \widehat{C}_{\alpha} | X_{n+1} \in \mathcal{R}(x)) \ge 1 - \alpha$ 

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.

## **CP-MDA** with Exact masking



# CQR-MDA with exact masking in words

- Split the training set into a proper training set and calibration set
- 2. Train the imputation function on the proper training set
- 3. Impute the proper training set
- 4. Train the quantile regressors on the imputed proper training set
- 5. For a test point  $(X^{(n+1)}, M^{(n+1)})$ :

5.1 For each  $j \in \llbracket 1, d \rrbracket$  s.t.  $M_j^{(n+1)} = 1$ , set  $\tilde{M}_j^{(k)} = 1$  for k in Cal s.t.  $M^{(k)} \subset M^{(n+1)}$ 



- 5.2 Impute the new calibration set
- 5.3 Compute the calibration correction, i.e.  $q_{1-\alpha}(S)$
- 5.4 Impute the test point
- 5.5 Predict with the quantile regressors and the correction previously obtained,  $q_{1-\alpha}(S)$

# **CP-MDA-Nested**









# CQR-MDA with nested masking in words

- 1. For a test point  $(X^{(n+1)}, M^{(n+1)})$ :
  - 1.1 Set  $\tilde{M}^{(k)} = \max(M^{(k)}, M^{(n+1)})$  for k in the calibration set
  - 1.2 Impute the new calibration set
  - 1.3 For each augmented calibration point k:
    - 1.3.1 Get its score  $S^{(k)}$

 $\begin{array}{c} \begin{array}{c} \text{Impute-then-predict on the augmented test point} \\ 1.3.2 & (X^{(n+1)}, \tilde{M}^{(k)}), \text{ giving:} \quad \widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),k}) \text{ and} \\ & \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k}) \end{array}$ 

1.3.3 Compute the corrected prediction interval:  $[\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),k}) - S^{(k)}; \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k}) + S^{(k)}] := [Z_{inf}^{(k)}; Z_{sup}^{(k)}]$ 1.4 Compute the quantiles  $q_{\alpha}(\{Z_{inf}^{(k)}\}_{k\in\text{Cal}})$  and  $q_{1-\alpha}(\{Z_{sup}^{(k)}\}_{k\in\text{Cal}})$ 1.5 Predict  $[q_{\alpha}(\{Z_{inf}^{(k)}\}_{k\in\text{Cal}}); q_{1-\alpha}(\{Z_{sup}^{(k)}\}_{k\in\text{Cal}})]$ 

	3	NA		NA		1	
$ ilde{x}^{(1)}$	-1	NA	N	IA	1		
$ ilde{x}^{(2)}$	4	NA	N	IA	2		
$ ilde{x}^{(3)}$	5	NA	N	IA	NA		
$ ilde{x}^{(4)}$	0	NA	N	IA	1		

3	NA	NA	1
3	NA	NA	1
3	NA	NA	NA
3	NA	NA	1

# Summary of CP-MDA



calibration set

