Introduction to Conformal Prediction
Extension to missing values

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Introduction to (Split) Conformal Prediction

Standard Split Conformal Prediction for Mean-Regression

Improving Adaptiveness: Conformalized Quantile Regression

Generalized SCP Framework

Take-home-messages and open directions

Quantifying Predictive Uncertainty with Missing Values

Conclusion

Setting

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables
- n training samples $\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n}$
- 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

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

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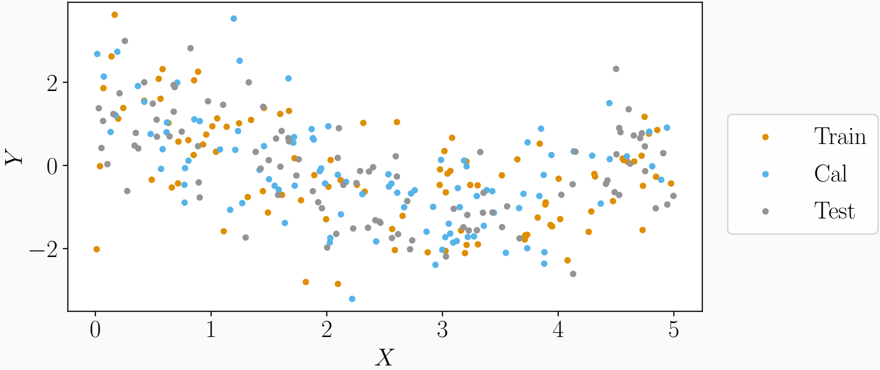
Split Conformal Prediction (SCP)[1,2,3]: toy example

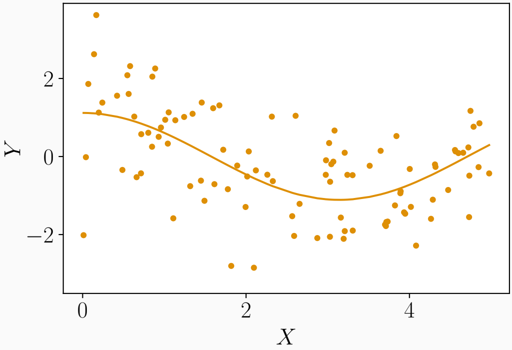


[1]Vovk et al. (2005), *Algorithmic Learning in a Random World*

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

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

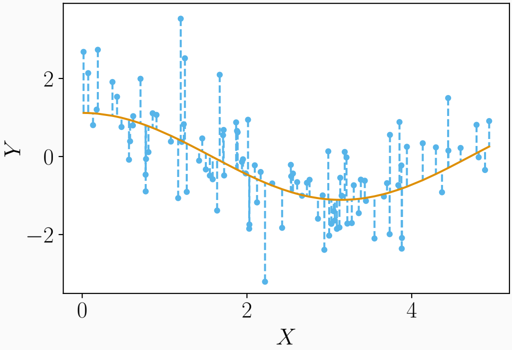
Split Conformal Prediction (SCP)[1,2,3]: training step



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

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



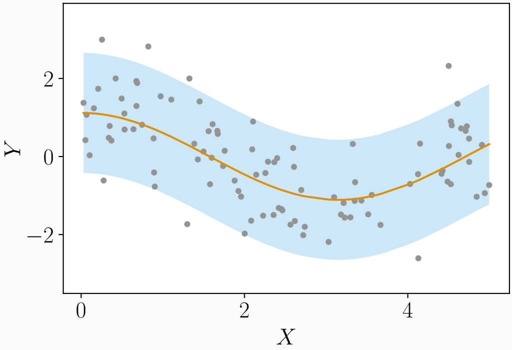
- Predict with $\hat{\mu}$
- Get the $|\text{residuals}|$
- Compute the $(1-\alpha)$ empirical quantile of the $|\text{residuals}| \cup \{+\infty\}$, noted $q_{1-\alpha}(\text{residuals})$

[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]: prediction step



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

[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*
[2] Papadopoulos et al. (2002), *Inductive Confidence Machines for Regression*, ECML
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Standard mean-regression SCP: formally

1. Split randomly the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
2. Train your algorithm on the proper training set to obtain $\hat{A}$
3. On the calibration set, get prediction values with $\hat{A}$
4. Obtain a set of $\#\mathrm{Cal} + 1$ conformity scores:

$$\mathcal{S} = \{S^{(i)} = |\hat{A}\left(X^{(i)}\right) - Y^{(i)}|, i \in \mathrm{Cal}\} \cup \{+\infty\}$$

(+ worst-case scenario)

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

$$\widehat{C}_\alpha\left(X^{(n+1)}\right) = \left[\hat{A}\left(X^{(n+1)}\right) - q_{1-\alpha}(\mathcal{S}); \hat{A}\left(X^{(n+1)}\right) + q_{1-\alpha}(\mathcal{S})\right]$$

SCP theoretical foundation

Definition (Exchangeability)

$\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n}$ are exchangeable if for any permutation σ of $[\![1, n]\!]$ we have:

$$\begin{aligned} & \mathcal{L}\left(\left(X^{(1)}, Y^{(1)}\right), \ldots, \left(X^{(n)}, Y^{(n)}\right)\right) \\ = \quad & \mathcal{L}\left(\left(X^{(\sigma(1))}, Y^{(\sigma(1))}\right), \ldots, \left(X^{(\sigma(n))}, Y^{(\sigma(n))}\right)\right), \end{aligned}$$

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 $\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n+1}$ *are exchangeable (or i.i.d.). SCP applied on* $\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha\left(X^{(n+1)}\right)$ *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 $\left\{S^{(i)}\right\}_{i \in \mathrm{Cal}}$ *are a.s. distinct:*

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

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

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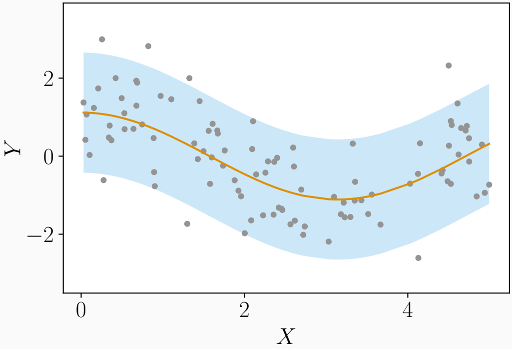
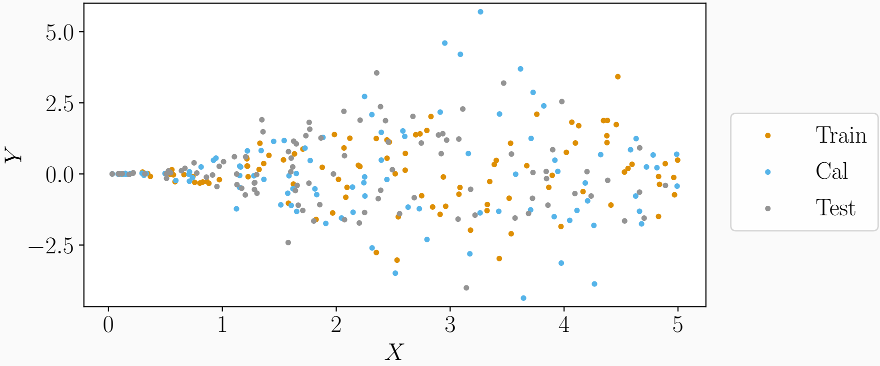
Standard mean-regression SCP is not adaptive



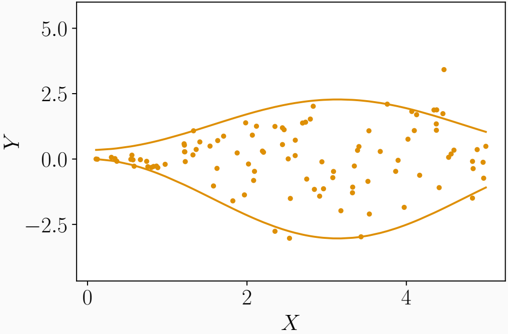
- Predict with $\hat{\mu}$
- Build $\widehat{C}_\alpha(x)$:
  $[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$

Conformalized Quantile Regression (CQR)[4]



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

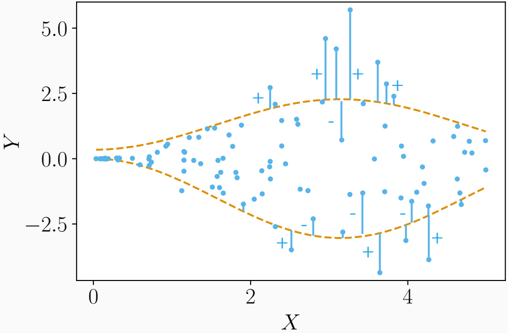
Conformalized Quantile Regression (CQR)[4]



- Learn (or get) $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$

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

Conformalized Quantile Regression (CQR)[4]



- Predict with $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$
- Get the scores $\mathcal{S} = \left\{ S^{(i)} \right\}_{\mathrm{Cal}} \cup \{+\infty\}$
- Compute the $(1-\alpha)$ empirical quantile of $\mathcal{S}$, noted $q_{1-\alpha}(\mathcal{S})$

$$\hookrightarrow \quad S^{(i)} := \max\left\{ \widehat{QR}_{\alpha/2}\left(X^{(i)}\right) - Y^{(i)}, Y^{(i)} - \widehat{QR}_{1-\alpha/2}\left(X^{(i)}\right) \right\}$$

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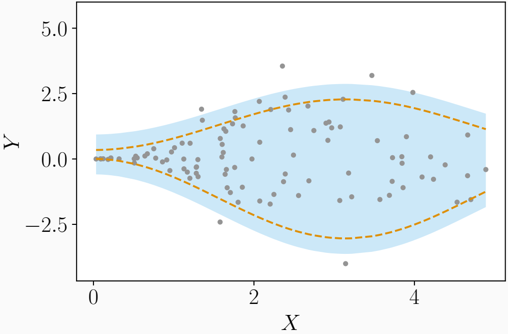
Conformalized Quantile Regression (CQR)[4]



- Predict with $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$

- Build

$$\widehat{C}_\alpha(x) = [\widehat{QR}_{\alpha/2}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{QR}_{1-\alpha/2}(x) + q_{1-\alpha}(\mathcal{S})]$$

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

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Generalization: SCP is defined by the conformity scores

1. Split randomly the training data into a proper training set (size $\#\mathrm{Tr}$) and a calibration set (size $\#\mathrm{Cal}$)
2. Train your algorithm on the proper training set to obtain $\hat{A}$
3. On the calibration set, obtain $\#\mathrm{Cal} + 1$ conformity scores

$$\mathcal{S} = \{S^{(i)} = \mathrm{s}\left(X^{(i)}, Y^{(i)}\right), i \in \mathrm{Cal}\} \cup \{+\infty\}$$

Ex 1: $\mathrm{s}(x, y) = |\hat{A}(x) - y|$ in mean-regression with standard scores

Ex 2: $\mathrm{s}(x, y) = \max\left(\widehat{QR}_{\alpha/2}(x) - y, y - \widehat{QR}_{1-\alpha/2}(x)\right)$ 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

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

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

SCP: theoretical guarantees generalized

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Theorem

Suppose $\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n+1}$ *are exchangeable (or i.i.d.). SCP applied on* $\left(X^{(i)}, Y^{(i)}\right)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha\left(X^{(n+1)}\right)$ *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 $\left\{S^{(i)}\right\}_{i \in \mathrm{Cal}}$ *are a.s. distinct:*

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

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

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SCP: summary

Split conformal prediction is simple to compute and works:

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

Two interests:

- quantify the uncertainty of the underlying model $\hat{A}$
- output predictive regions

Note that the theoretical guarantee is **marginal** over the joint distribution of (X, Y), and **not conditional**. That is, there is no guarantee that for any $x \in \mathbb{R}$:

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

Challenges and open directions (non-exhaustive references)

1. Providing a form of conditional guarantee
2. Tradeoffs between computational cost and statistical efficiency (i.e. variability of the estimators, *efficiency* of the predictive sets)
3. Going beyond the exchangeability assumption

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

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Missing values: ubiquitous in data science practice

Y	X_1	X_2	X_3	X_4	X_5	X_6
22.42	0.55	0.67	0.03	0.75	0.05	0.05
8.26	0.72	0.18	0.55	0.05	0.73	0.50
~~19.41~~	~~0.60~~	~~0.58~~	~~NA~~	~~NA~~	~~NA~~	~~0.40~~
19.75	0.54	0.43	0.96	0.77	0.06	0.66
~~7.32~~	~~NA~~	~~0.19~~	~~NA~~	~~0.02~~	~~0.83~~	~~0.04~~
~~13.55~~	~~0.65~~	~~0.69~~	~~0.50~~	~~0.15~~	~~NA~~	~~0.87~~
20.75	0.43	0.74	0.61	0.72	0.52	0.35
~~9.26~~	~~0.89~~	~~NA~~	~~0.84~~	~~0.01~~	~~0.73~~	~~NA~~
~~9.68~~	~~0.963~~	~~0.45~~	~~0.65~~	~~0.04~~	~~0.06~~	~~NA~~

If each entry has a probability 0.01 of being missing:

$$d = 6 \rightarrow \approx 94\% \text{ of rows kept}$$

$$d = 300 \rightarrow \approx 5\% \text{ of rows kept}$$

One of the **ironies of Big Data** *is that missing data play an ever more significant role.*[5]

[5] Zhu et al. (2019), *High-dimensional PCA with heterogeneous missingness*, JRSS B

Handling missing values depends on pattern and mechanism

- $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ random variables.
- $M \in \{0,1\}^d$ is defined as $M_j = 1 \Leftrightarrow X_j$ is missing.
  M is called the **mask** or the **missing pattern**.

Example

We observe $(\texttt{NA}, 6, 2)(-1, \texttt{NA}, 2)(-1, \texttt{NA}, \texttt{NA})$. Then
$m = (1, 0, 0) m = (0, 1, 0) m = (0, 1, 1)$.

There are 2^d **patterns** (statistical and computational challenges).

- Three **mechanisms**[6] can generate missing values.
  $\hookrightarrow$ **Missing Completely At Random** (MCAR):
  $\mathbb{P}(M = m|X) = \mathbb{P}(M = m)$ for all $m \in \{0,1\}^d$. $M \perp\!\!\!\perp X$,
  missingness does not depend on the variables.

[6] Rubin (1976), *Inference and missing data*, Biometrika

Supervised learning with missing values

Impute-then-regress procedures are widely used.

1. Replace `NA` using an imputation function ϕ (e.g. the mean).
2. Train your algorithm (Random Forest, Neural Nets, etc.) on the imputed data: $\left\{ \underbrace{\phi\left(X^{(i)}_{\mathrm{obs}(M^{(i)})}, M^{(i)}\right)}_{\text{imputed } X^{(i)}}, Y^{(i)} \right\}_{k=1}^{n}$.

✓: Le Morvan et al. (2021)[7] show that for any deterministic imputation and universal learner this procedure is Bayes-consistent.

✗: Ayme et al. (2022)[8] show that even for very **simple distributions** (linear model, Gaussian noise), may suffer from **curse of dimensionality**.

[7] Le Morvan et al. (2021), *What's a good imputation to predict with missing values?*, NeurIPS

[8] Ayme et al. (2022), *Near-optimal rate of consistency for linear models with missing values*, ICML

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Impute-then-regress+conformalization is marginally valid

To apply conformal prediction we need **exchangeable** data.

Lemma (Exchangeability after imp., Zaffran et al., 2023)

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

Then, for **any missing mechanism**, **for almost all imputation function** ϕ*:*

$\left(\phi\left(X^{(i)}_{obs(M^{(i)})}, M^{(i)}\right), Y^{(i)}\right)_{i=1}^{n}$ *are* **exchangeable**.

$\Rightarrow$ Conformal prediction applied on an imputed data set still enjoys marginal guarantees[9]:

$$\mathbb{P}\left(Y \in \widehat{C}_\alpha\left(X_{\mathrm{obs}(M)}, M\right)\right) \geq 1 - \alpha.$$

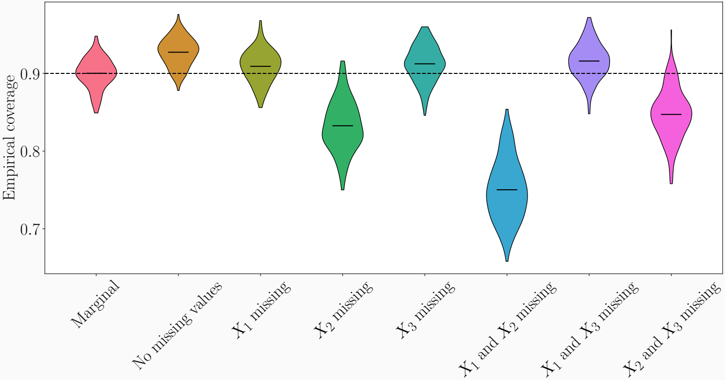
Even if the imputation is not accurate, the guarantee will hold.

[9]The upper bound also holds under continuously distributed scores.

CQR performances on an illustrative example

$$Y = \beta^T X + \varepsilon,$$

with $\beta = (1, 2, -1)^T$, $\varepsilon \perp\!\!\!\perp X$ and X and ε are Gaussian.



Warning: the predictive intervals cover properly **marginally**, but suffer from high **disparities depending on the missing patterns**.

Missing values induce heteroskedasticity

Theoretical study of the Gaussian linear model ($Y = \beta^T X + \varepsilon$) generalizes:

Proposition (Oracle intervals under the Gaussian lin. mod.)

$$\mathcal{L}_\alpha^*(m) = 2 \times q_{1-\alpha/2}^{\mathcal{N}(0,1)} \times \sqrt{\beta_{\mathrm{mis}(m)}^T \Sigma_{\mathrm{mis|obs}}^m \beta_{\mathrm{mis}(m)} + \sigma_\varepsilon^2}.$$

- Even with an homoskedastic noise, missingness generates heteroskedasticity
- **The uncertainty increases when missing values are associated with larger regression coefficients (i.e. the most predictive variables)**

Goal: validity conditionally to the mask

Goal: for any $m \in \mathcal{M} \subset \{0,1\}^d$:

$$\mathbb{P}\left(Y \in \widehat{C}_\alpha\left(X_{\mathrm{obs}(M)}, M\right)|M = m\right) \geq 1 - \alpha.$$

Motivation: equity, first-step-towards-conditional.

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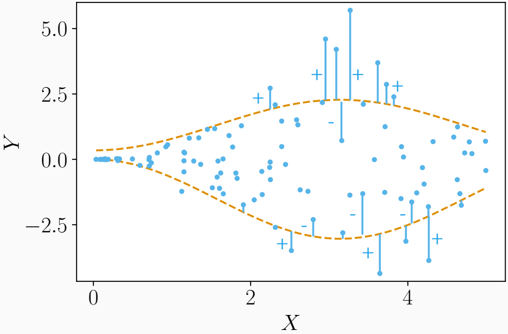
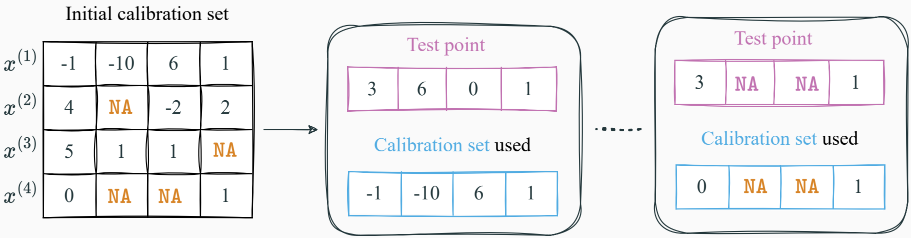
Issue during the calibration step



- Predict with $\widehat{QR}_{\alpha/2}$ and $\widehat{QR}_{1-\alpha/2}$
- Get the scores $\mathcal{S} = \left\{S^{(i)}\right\}_{\mathrm{Cal}} \cup \{+\infty\}$
- Compute the $(1-\alpha)$ empirical quantile of $\mathcal{S}$, noted $q_{1-\alpha}(\mathcal{S})$

Infeasible solution: splitting the calibration set[10] for each mask



[10] Romano et al. (2020), *With Malice Toward None: Assessing Uncertainty via Equalized Coverage*, Harvard Data Science Review

Missing data augmentation of the calibration set

Test point

3	NA	NA	1

Initial calibration set

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

Calibration set used

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$				
$\tilde{x}^{(4)}$	0	NA	NA	1

$$\hookrightarrow \quad S^{(i)} := \max\left\{\widehat{QR}_{\alpha/2}\left(\tilde{X}^{(i)}\right) - Y^{(i)}, Y^{(i)} - \widehat{QR}_{1-\alpha/2}\left(\tilde{X}^{(i)}\right)\right\}$$

CQR-MDA with exact masking in words

1. 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 $\left(X^{(n+1)}, M^{(n+1)}\right)$:

3	NA	NA	1

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$				
$\tilde{x}^{(4)}$	0	NA	NA	1

   5.1 For each $j \in [\![1, d]\!]$ s.t. $M_j^{(n+1)} = 1$, set $\tilde{M}_j^{(i)} = 1$ for i in Cal s.t. $M^{(i)} \subset M^{(n+1)}$
   5.2 Impute the new calibration set
   5.3 Compute the calibration correction, i.e. $q_{1-\alpha}(\mathcal{S})$
   5.4 Impute the test point
   5.5 Predict with the quantile regressors and the correction previously obtained, $q_{1-\alpha}(\mathcal{S})$

Mask conditional validity

Theorem (Zaffran et al., 2023)

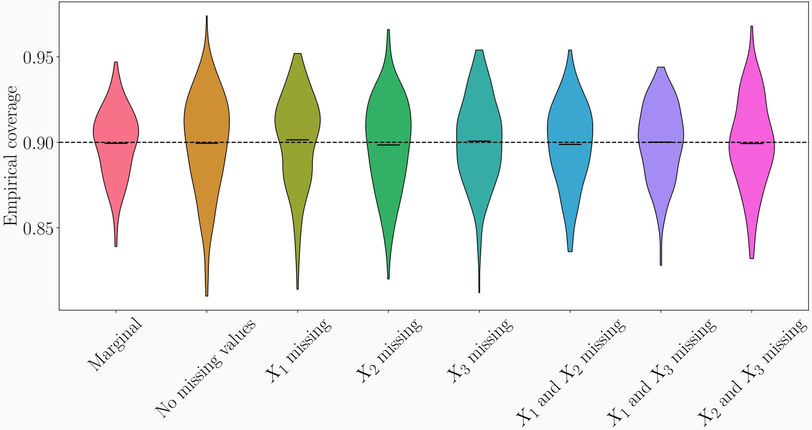
If the data is exchangeable and MCAR, then for almost all imputation function the proposed methodology is such that for any $m \in \{0,1\}^d$*:*

$$\mathbb{P}\left(Y \in \widehat{C}_\alpha\left(X_{obs(M)}, M\right) | M = m\right) \geq 1 - \alpha,$$

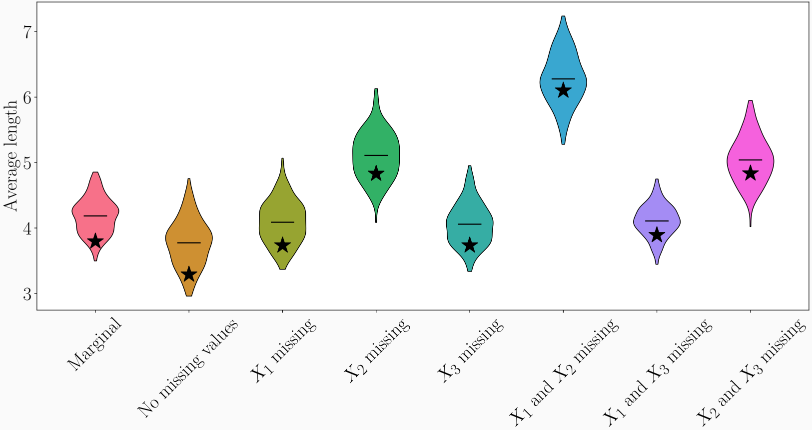
and if additionally the scores are almost surely distinct:

$$\mathbb{P}\left(Y \in \widehat{C}_\alpha\left(X_{obs(M)}, M\right) | M = m\right) \leq 1 - \alpha + \frac{1}{1 + \#\mathrm{Cal}^{\mathrm{m}}}.$$

Empirical coverages



Empirical lengths



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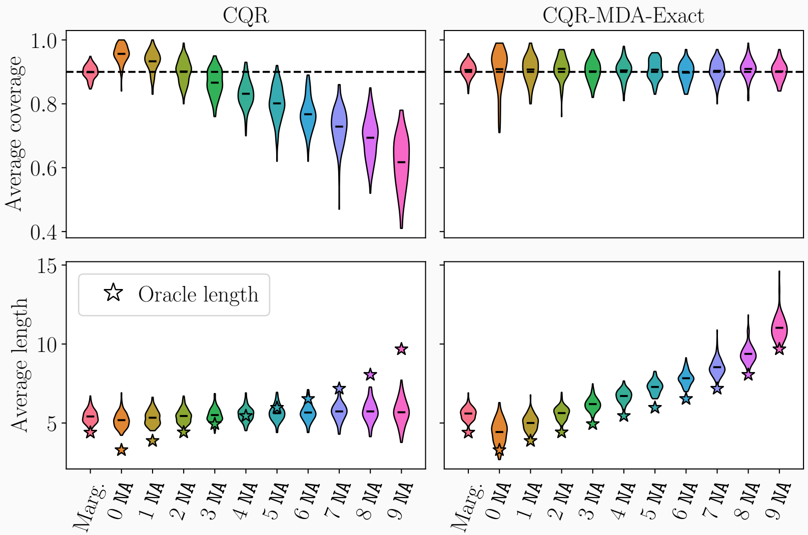
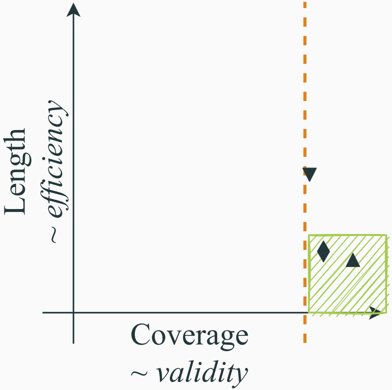
Some settings

- Imputation by iterative ridge ($\sim$ conditional expectation)
- **Concatenate the mask in the features**
- Neural network, fitted to minimize the pinball loss
- (Semi)-synthetic experiments:
  - MCAR missing values, with probability 20%
  - 100 repetitions

Synthetic experiments (Gaussian linear model, $d = 10$)



Before more experiments, visualisation



- ♦ : marginal coverage, i.e.

  $\mathbb{P}(Y \in \hat{C}_\alpha(X, M))$

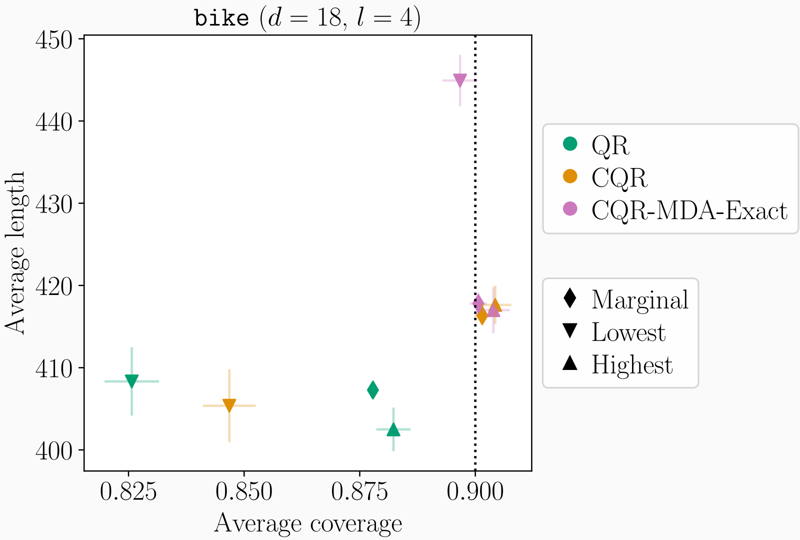
- ▼ : lowest coverage, i.e.

  $\min_{m \in \mathcal{M}} \mathbb{P}(Y \in \hat{C}_\alpha(X, m) | M = m)$

- ▲ : highest coverage, i.e.

  $\max_{m \in \mathcal{M}} \mathbb{P}(Y \in \hat{C}_\alpha(X, m) | M = m)$

Semi-synthetic experiments



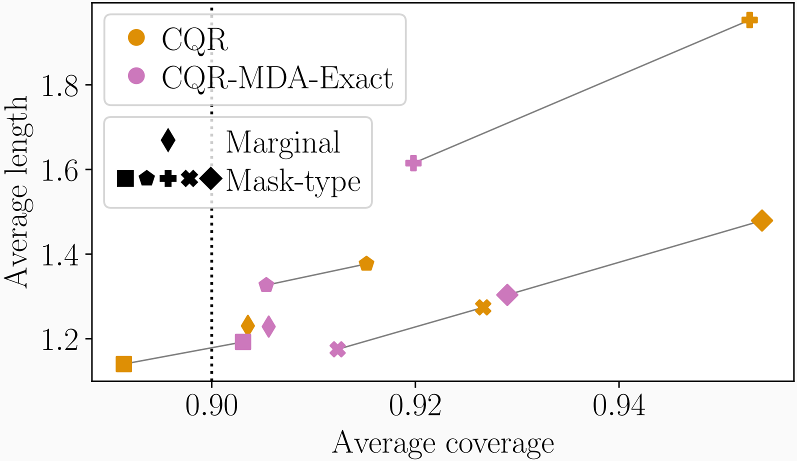
TraumaBase®: decision support for trauma patients

- 30 hospitals
- More than 30 000 trauma patients
- 4 000 new patients per year
- 250 continuous and categorical variables
  $\hookrightarrow$ Many useful statistical tasks

Predict the level of platelets upon arrival at hospital, given 7 covariates chosen by medical doctors.

These covariates are not always observed: from 0% to 24% of missing values by features, with a total average of 7%.

Real data experiment: TraumaBase®, critical care medicine



Introduction to (Split) Conformal Prediction

Quantifying Predictive Uncertainty with Missing Values

Conclusion

Extensions

- Consistency of universal quantile learner when chained with almost any imputation function.
- CP-MDA-Nested link to CP-MDA-Nested, an algorithm which does not discard any calibration point.

Take-home-messages

- 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).

Thank you!

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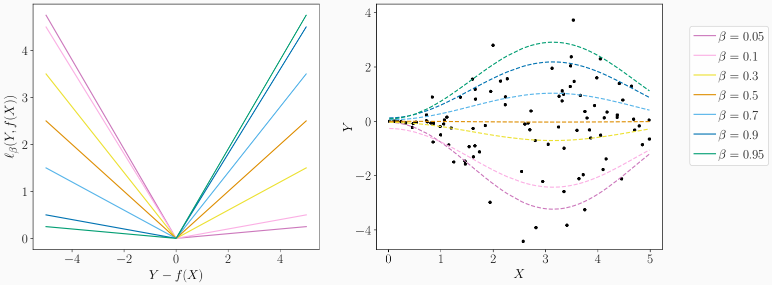
Appendix

Quantile regression

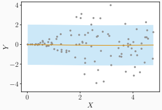
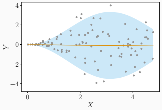
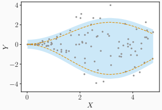


Warning

No theoretical guarantee with a finite sample

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

SCP: what choices for the regression scores?

	Standard SCP Vovk et al. (2005)	**Locally weighted SCP** Lei et al. (2018)	**CQR** Romano et al. (2019)
$s(X, Y)$	$\lvert \hat{A}(X) - Y \rvert$	$\frac{\lvert \hat{A}(X) - Y \rvert}{\hat{\rho}(X)}$	$\max(\widehat{QR}_{\alpha/2}(X) - Y, Y - \widehat{QR}_{1-\alpha/2}(X))$
$\widehat{C}_\alpha(x)$	$\left[\hat{A}(x) \pm q_{1-\alpha}(\mathcal{S})\right]$	$\left[\hat{A}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)\right]$	$[\widehat{QR}_{\alpha/2}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{QR}_{1-\alpha/2}(x) + q_{1-\alpha}(\mathcal{S})]$
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 in classification
(from C. Boyer and M. Zaffran tutorial)

SCP in classification

- $Y^{(i)} \in \{1, \ldots, C\}$ (C classes)
- $\hat{A}(X) = (\hat{p}_1(X), \ldots, \hat{p}_C(X))$ (estimated probabilities)
- Score of the i-th calibration point: $S^{(i)} = 1 - (\hat{A}\left(X^{(i)}\right))_{Y^{(i)}}$
- For a new point $X^{(n+1)}$, return

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

SCP in classification in practice

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

- Scores on the calibration set

$\mathrm{Cal}^{(i)}$										
$\hat{p}_{\text{dog}}\left(X^{(i)}\right)$	0.95	0.90	0.85	0.15	0.15	0.20	0.15	0.15	0.25	0.20
$\hat{p}_{\text{tiger}}\left(X^{(i)}\right)$	0.02	0.05	0.10	0.60	0.55	0.50	0.45	0.40	0.35	0.45
$\hat{p}_{\text{cat}}\left(X^{(i)}\right)$	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

- $q_{1-\alpha}(\mathcal{S}) = 0.65$ $\qquad \lceil 0.9 \times (10+1) \rceil = 10$
- $\hat{A}\left(X^{(n+1)}\right) = (0.05, 0.60, 0.35)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{"dog"}) = 0.95$ $\qquad$ "dog" $\notin \widehat{C}_\alpha\left(X^{(n+1)}\right)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{"tiger"}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$
    "tiger" $\in \widehat{C}_\alpha\left(X^{(n+1)}\right)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{"cat"}) = 0.65 \leq q_{1-\alpha}(\mathcal{S})$ $\qquad$ "cat" $\in \widehat{C}_\alpha\left(X^{(n+1)}\right)$
- $\widehat{C}_\alpha\left(X^{(n+1)}\right) = \{$"tiger", "cat"$\}$

SCP in classification in practice

Ex: $Y^{(i)} \in \{\text{“dog”}, \text{“tiger”}, \text{“cat”}\}$, with $\alpha = 0.1$

- Scores on the calibration set

$\mathrm{Cal}^{(i)}$										
$\hat{p}_{\text{dog}}(X^{(i)})$	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

- $q_{1-\alpha}(\mathcal{S}) = 0.45$ $\lceil 0.9 \times (10+1) \rceil = 10$
- $\hat{A}\left(X^{(n+1)}\right) = (0.05, 0.60, 0.35)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{“dog”}) = 0.95$ “dog” $\notin \widehat{C}_\alpha\left(X^{(n+1)}\right)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{“tiger”}) = 0.40 \leq q_{1-\alpha}(\mathcal{S})$
    “tiger” $\in \widehat{C}_\alpha\left(X^{(n+1)}\right)$
  - $\hookrightarrow s(\hat{A}\left(X^{(n+1)}\right), \text{“cat”}) = 0.65$ “cat” $\notin \widehat{C}_\alpha\left(X^{(n+1)}\right)$
- $\widehat{C}_\alpha\left(X^{(n+1)}\right) = \{\text{“tiger”}\}$

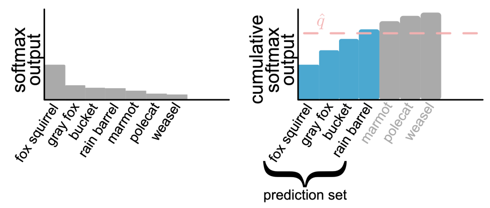
SCP in classification: comments on the naive version

- Facts about the previous method
  - prediction sets with the smallest average size
  - undercover hard subgroups
  - overcover easy ones
- Other types of scores can be used to improve the conditional coverage (as in regression with CQR or localized)

SCP in classification: Adaptive Prediction Sets

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

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



SCP in classification in practice: Adaptive Prediction Sets

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

- Scores on the calibration set

$\mathrm{Cal}^{(i)}$										
$\hat{p}_{\text{dog}}\left(X^{(i)}\right)$	0.95	0.90	0.85	0.05	0.05	0.05	0.10	0.25	0.10	0.15
$\hat{p}_{\text{tiger}}\left(X^{(i)}\right)$	0.02	0.05	0.10	0.85	0.80	0.75	0.75	0.40	0.30	0.30
$\hat{p}_{\text{cat}}\left(X^{(i)}\right)$	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

- $q_{1-\alpha}(\mathcal{S}) = 0.95$
- Ex 1: $\hat{A}\left(X^{(n+1)}\right) = (0.05, 0.45, 0.5), r^\star = 2$

  $\widehat{C}_\alpha\left(X^{(n+1)}\right) = \{$"tiger", "cat"$\}$
- Ex 2: $\hat{A}\left(X^{(n+1)}\right) = (0.03, 0.95, 0.02), r^\star = 1$

  $\widehat{C}_\alpha\left(X^{(n+1)}\right) = \{$"tiger"$\}$

Jackknife/cross-val (from C. Boyer and M. Zaffran tutorial)

Beyond the limitations of SCP

- SCP is computationally attractive: it only requires fitting the model one time
- Problem: it sacrifices statistical efficiency
  - requiring splitting the data into training and calibration datasets

$\rightsquigarrow$ Full (or transductive) conformal prediction
  - avoids data splitting
  - at the cost of many more model fits

- Historically, full conformal prediction was developed first
- Idea: we know that the true label $Y^{(n+1)}$ lives somewhere in $\mathcal{Y}$ so if we loop over all possible $y \in \mathcal{Y}$, then we will eventually hit the data point $(X^{(n+1)}, Y^{(n+1)})$, which is statistically plausible with the first n data points
- Hence the name as full conformal prediction directly computes this loop

Full conformal prediction

Method: for a candidate $(X^{(n+1)}, y)$,

1. Get $\hat{A}_y$ by training on $\{(X^{(1)}, Y^{(1)}), \ldots, (X^{(n)}, Y^{(n)})\} \cup \{(X^{(n+1)}, y)\}$
2. Scores

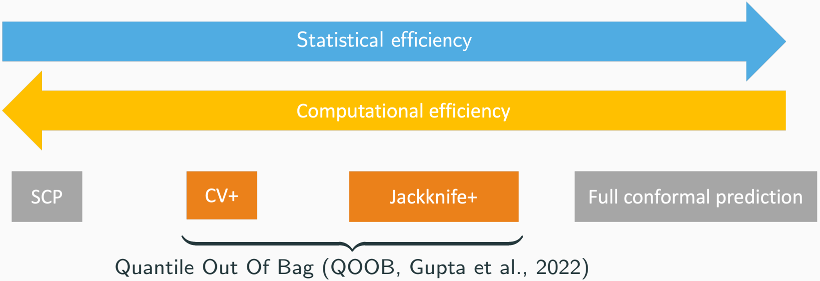
$$\mathcal{S} = \left\{ s(\hat{A}_y \left(X^{(i)}, Y^{(i)} \right) \right\} \cup \{ s(\hat{A}_y \left(X^{(n+1)} \right), y) \}$$

3. $y \in \widehat{C}_\alpha \left(X^{(n+1)} \right)$ if $s(\hat{A}_y \left(X^{(n+1)} \right), y) \leq q_{1-\alpha}(\mathcal{S})$

✓ Theoretical guarantees (provided that the learining algorithm handles exchangeable training data in a symmetric way)

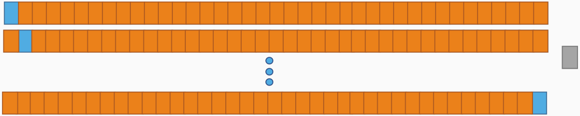
✗ Computationally costly: not used in practice

Other methods for conformal prediction



Jackknife: naive predictive interval

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



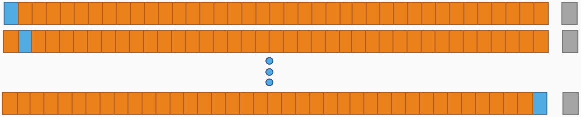
- $\mathcal{D}^n = \left\{ \left(X^{(1)}, Y^{(1)}\right), \dots, \left(X^{(n)}, Y^{(n)}\right) \right\}$ training data
- Get $\hat{A}^{-i}$ by training on $\mathcal{D}^n \setminus \left(X^{(i)}, Y^{(i)}\right)$
- LOO scores $\mathcal{S} = \left\{ \left| \hat{A}^{-i}\left(X^{(i)}\right) - Y^{(i)} \right| \right\}_i \cup \{+\infty\}$ (in standard reg)
- Get $\hat{A}$ by training on $\mathcal{D}^n$
- Build the predictive interval: $\left[\hat{A}\left(X^{(n+1)}\right) \pm q_{1-\alpha}(\mathcal{S}) \right]$

Warning

No guarantee on the prediction of $\hat{A}$ with scores based on $(\hat{A}^{-i})_i$

Jackknife+ (Barber et al., 2021b)

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



- $\mathcal{D}^n = \left\{ \left(X^{(1)}, Y^{(1)}\right), \dots, \left(X^{(n)}, Y^{(n)}\right) \right\}$ training data
- Get $\hat{A}^{-i}$ by training on $\mathcal{D}^n \setminus \left(X^{(i)}, Y^{(i)}\right)$
- LOO predictions (in standard reg)
  $$\mathcal{S}_{\text{up/down}} = \left\{ \hat{A}^{-i}\left(X^{(n+1)}\right) \pm \left| \hat{A}^{-i}\left(X^{(i)}\right) - Y^{(i)} \right| \right\}_i \cup \{\pm\infty\}$$
- Build the predictive interval: $\left[q_{\alpha/2}(\mathcal{S}_{\text{down}}); q_{1-\alpha/2}(\mathcal{S}_{\text{up}}) \right]$

Theorem

If $\mathcal{D}^n \cup (X^{(n+1)}, Y^{(n+1)})$ are exchangeable and the algorithm treats the data points symmetrically, then $\mathbb{P}(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right)) \geq 1 - 2\alpha$.

CV+ (Barber et al., 2021b)

- Based on cross-validation residuals
- $\mathcal{D}^n = \left\{ \left(X^{(1)}, Y^{(1)}\right), \dots, \left(X^{(n)}, Y^{(n)}\right) \right\}$ training data

1. Split $\mathcal{D}^n$ into K folds $F_1, \dots, F_K$
2. Get $\hat{A}^{-F_k}$ by training on $\mathcal{D}^n \setminus F_k$
3. Cross-val predictions (in standard reg)
   $$\mathcal{S}_{\text{up/down}} = \left\{ \left\{ \hat{A}^{-F_k}\left(X^{(n+1)}\right) \pm \left| \hat{A}_{-F_k}\left(X^{(i)}\right) - Y^{(i)} \right| \right\}_{i \in F_k} \right\}_k \cup \{\pm\infty\}$$
4. Build the predictive interval: $[q_\alpha(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

Theorem

Under data exchangeability and algorithm symmetry, then
$$\mathbb{P}(Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}\right)) \geq 1 - 2\alpha - \min\left(\frac{2(1-1/K)}{n/K+1}, \frac{1-K/n}{K+1}\right) \geq 1 - 2\alpha - \sqrt{2/n}.$$

CP-MDA-Nested

CP-MDA-Exact reminder

Test point

3	NA	NA	1

Initial calibration set

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

Calibration set used

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$				
$\tilde{x}^{(4)}$	0	NA	NA	1

What if we kept all individuals?

Test point

3	NA	NA	1

Initial calibration set

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

Calibration set used

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$	5	NA	NA	NA
$\tilde{x}^{(4)}$	0	NA	NA	1

Idea: modify the test point accordingly

Test point

3	NA	NA	1

Initial calibration set

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

Calibration set used

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$	5	NA	NA	NA
$\tilde{x}^{(4)}$	0	NA	NA	1

and

Temporary test points

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

CQR-MDA with nested masking in words

1. For a test point $(X^{(n+1)}, M^{(n+1)})$:

3	NA	NA	1

   1.1 Set $\tilde{M}^{(i)} = \max(M^{(i)}, M^{(n+1)})$ for i in the calibration set

$\tilde{x}^{(1)}$	-1	NA	NA	1
$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$	5	NA	NA	NA
$\tilde{x}^{(4)}$	0	NA	NA	1

   1.2 Impute the new calibration set

   1.3 For each augmented calibration point i:

      1.3.1 Get its score $S^{(i)}$

      1.3.2 Impute-then-predict on the augmented test point $(X^{(n+1)}, \tilde{M}^{(i)})$, giving: $\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),i})$ and $\widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),i})$

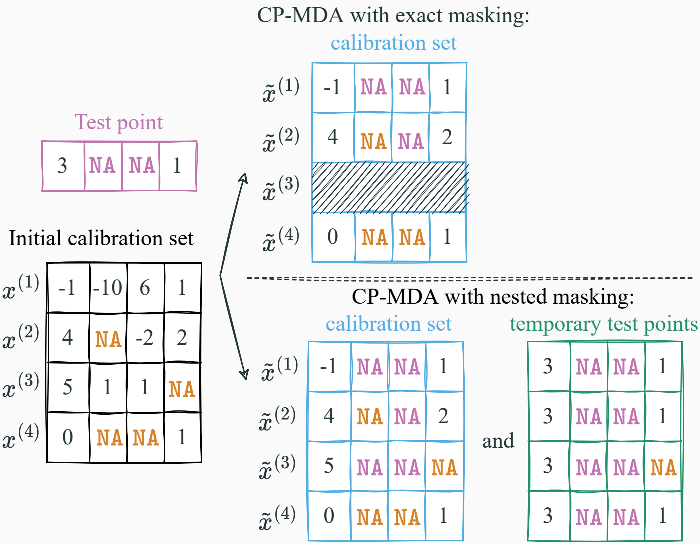
3	NA	NA	1
3	NA	NA	1
3	NA	NA	NA
3	NA	NA	1

      1.3.3 Compute the corrected prediction interval: $[\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),i}) - S^{(i)}; \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),i}) + S^{(i)}] := \left[Z_{\text{inf}}^{(i)}; Z_{\text{sup}}^{(i)}\right]$

   1.4 Compute the quantiles $q_\alpha(\{Z_{\text{inf}}^{(i)}\}_{i\in\mathrm{Cal}})$ and $q_{1-\alpha}(\{Z_{\text{sup}}^{(i)}\}_{i\in\mathrm{Cal}})$

   1.5 Predict $[q_\alpha(\{Z_{\text{inf}}^{(i)}\}_{i\in\mathrm{Cal}}); q_{1-\alpha}(\{Z_{\text{sup}}^{(i)}\}_{i\in\mathrm{Cal}})]$

Summary of CP-MDA



Towards asymptotic individualized coverage

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

$$g^*_{\beta,\Phi} \in \underset{g:\mathbb{R}^d \to \mathbb{R}}{\text{argmin}} \ \mathbb{E}\left[\rho_\beta(Y - g \circ \Phi(X_{\text{obs(M)}}, M))\right] := \mathcal{R}_{\beta,\phi}(g).$$

Comparison with: $\underset{f}{\text{argmin}} \ \mathbb{E}\left[\rho_\beta(Y - f(X_{\text{obs(M)}}, M))\right]$ *(informal)*.

Proposition (Pinball-consistency of an universal learner)

For almost all $\mathcal{C}^\infty$ imputation function Φ, the function $g^*_{\beta,\Phi} \circ \Phi$ is Bayes optimal for the pinball-risk of level β.

$\hookrightarrow$ any universally consistent algorithm for quantile regression trained on the data imputed by Φ is pinball-Bayes-consistent.

This is an extension of the result of Le Morvan et al. (2021).

Asymptotic conditional coverage of a universal quantile learner

Corollary

For any missing mechanism, for almost all $\mathcal{C}^\infty$ imputation function Φ, if $F_{Y|(X_{\mathrm{obs(M)}},M)}$ is continuous, a universally consistent quantile regressor trained on the imputed data set yields asymptotic conditional coverage.

$\hookrightarrow \mathbb{P}(Y \in \widehat{C}_\alpha(x) | X = x, M = m) \geq 1 - \alpha$ for any $m \in \mathcal{M}$ and any $x \in \mathbb{R}^d$, asymptotically with a super quantile learner.

$$d = 3$$

Data generation

$(X, Y) \in \mathbb{R}^3 \times \mathbb{R}$.

$Y = \beta X + \varepsilon$

with $\varepsilon \sim \mathcal{N}(0, 1)$, $\beta = (1, 2, -1)$ and

$$(X_1, X_2, X_3) \sim \mathcal{N}\left(\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 & 0.8 & 0.8 \\ 0.8 & 1 & 0.8 \\ 0.8 & 0.8 & 1 \end{pmatrix}\right).$$

All components of X each have a probability 0.2 of being missing, Completely At Random.

Simulation settings

- Method: CQR
- Basemodel: neural network
- 200 repetitions
  - `train size` of 250 points
  - `calibration size` of 250 points
  - `test size` of 2000 points

$d = 10$, with missing data augmentation

Data generation

$(X, Y) \in \mathbb{R}^{10} \times \mathbb{R}$.

$Y = \beta X + \varepsilon$

with $\varepsilon \sim \mathcal{N}(0, 1)$, $\beta = (1, 2, -1, 3, -0.5, -1, 0.3, 1.7, 0.4, -0.3)$

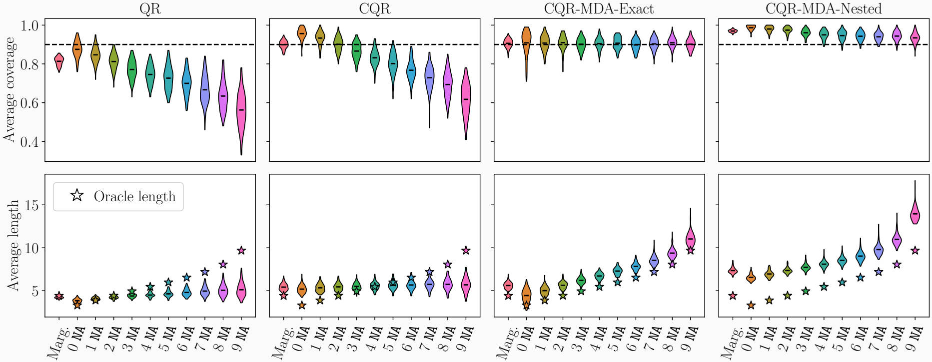
and $(X_1, \cdots, X_{10}) \sim \mathcal{N}\left(\begin{pmatrix} 1 \\ \vdots \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} 1 & 0.8 & \cdots & 0.8 \\ 0.8 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0.8 \\ 0.8 & \cdots & 0.8 & 1 \end{pmatrix}\right)$.

All components of X each have a probability 0.2 of being missing, Completely At Random.

Simulation settings

- Method: CQR
- Basemodel: neural network
- Imputation: iterative ($\approx$ conditional expectation)
- Mask as features: yes
- 100 repetitions
    - `train size` of 500 points
    - `calibration size` of 250 points
    - `test size` of 100 points for each pattern size, and 2000 for the marginal test set

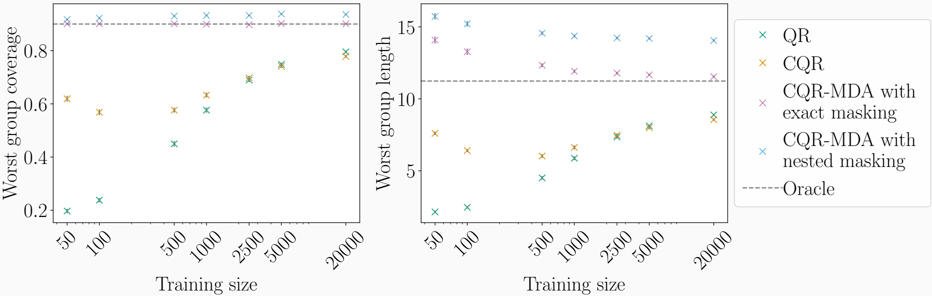
Results per pattern size



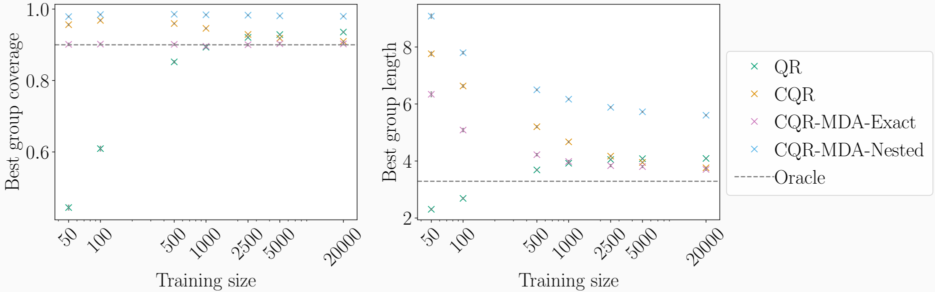
Simulation settings: varying training size

- Method: CQR
- Basemodel: neural network
- Imputation: iterative (≈ conditional expectation)
- Mask as features: yes
- 100 repetitions
  - `train size` varies
  - `calibration size` of 1000 points
  - `test size` of 2000 points

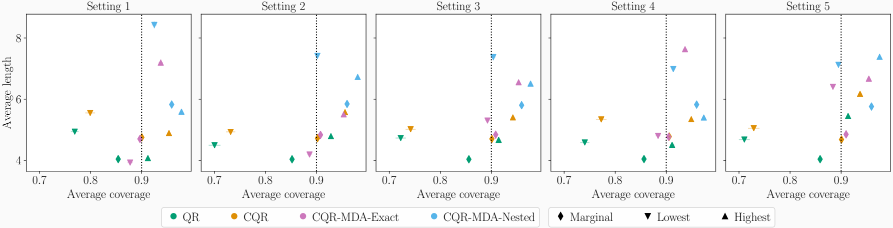
Results on the worst group



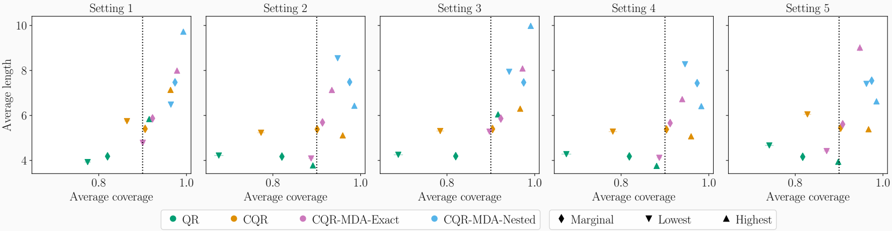
Results on the best group



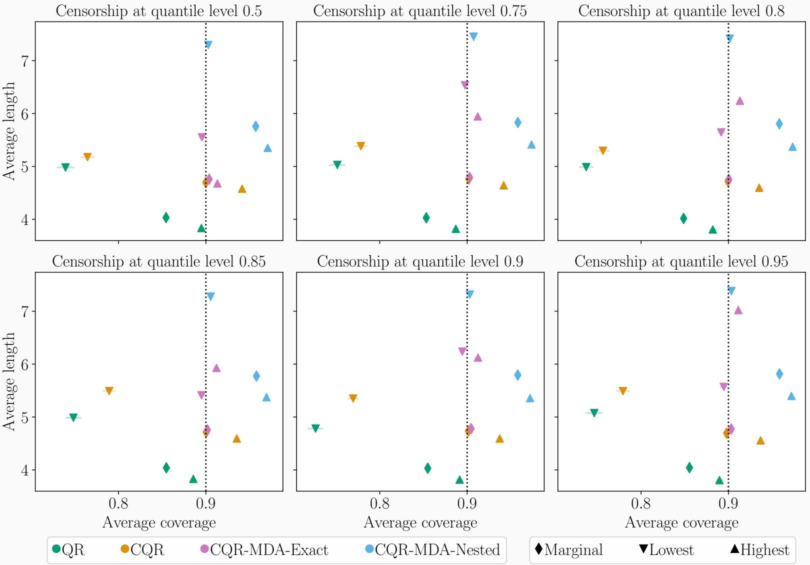
MAR missingness



MNAR self masked missingness

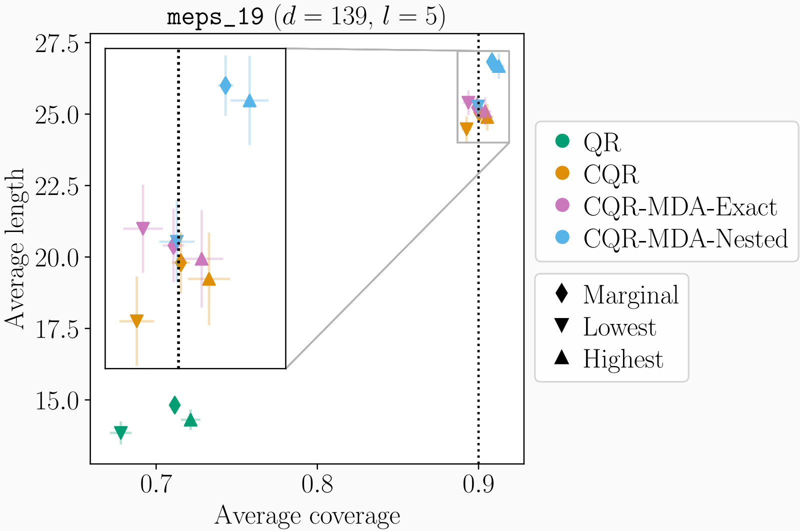


MNAR quantile censorship missingness

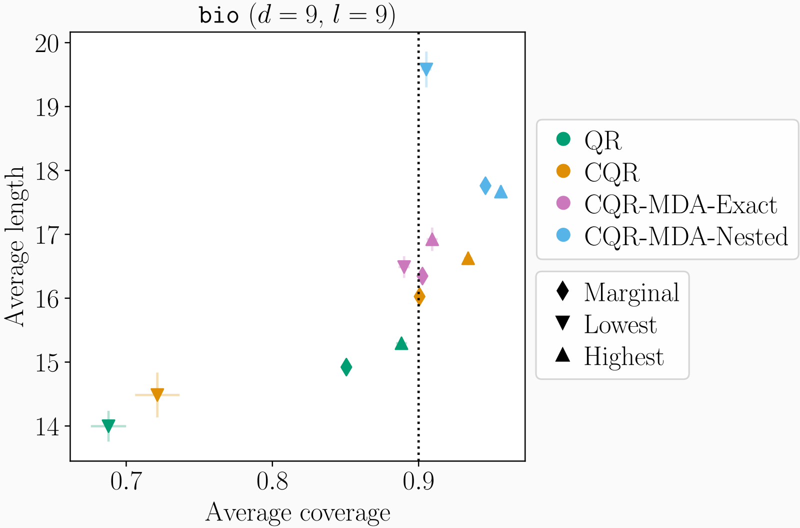


Semi-synthetic experiments with CQR-MDA-Nested

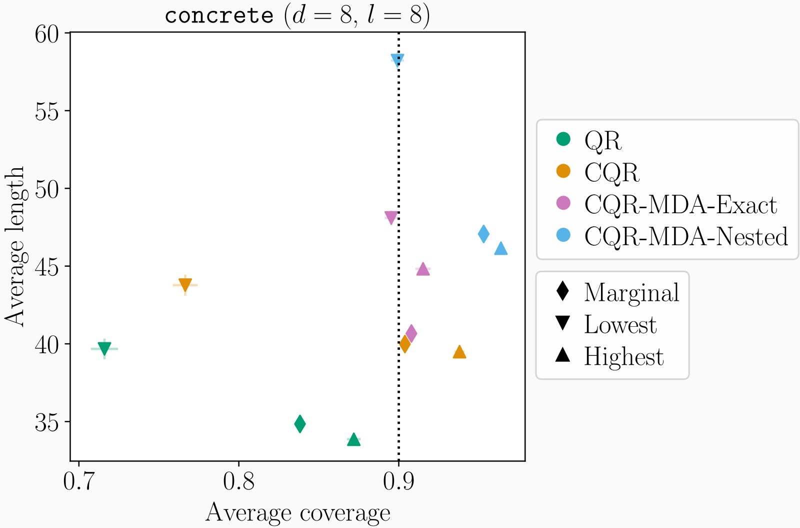
Semi-synthetic experiments with CQR-MDA-Nested



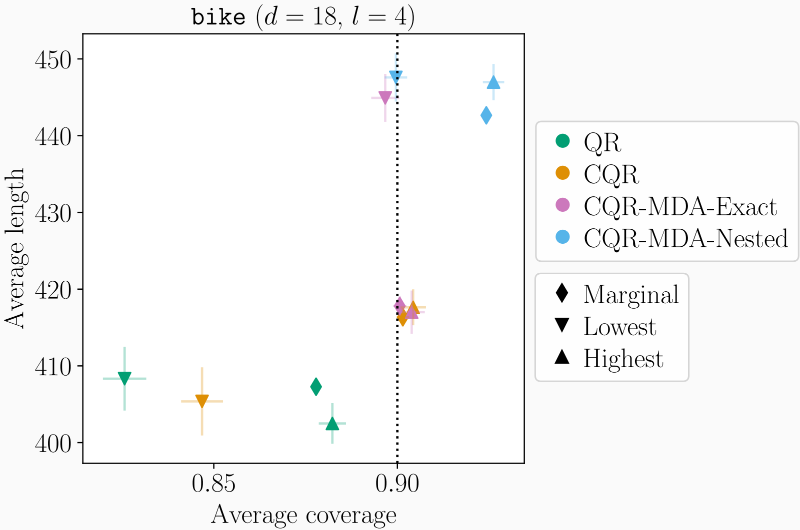
Semi-synthetic experiments with CQR-MDA-Nested



Semi-synthetic experiments with CQR-MDA-Nested



Semi-synthetic experiments with CQR-MDA-Nested



TraumaBase®

TraumaBase®: decision support for trauma patients

- 30 hospitals
- More than 30 000 trauma patients
- 4 000 new patients per year
- 250 continuous and categorical variables
  $\hookrightarrow$ Many useful statistical tasks

Predict the level of platelets upon arrival at hospital, given 7 covariates chosen by medical doctors.

These covariates are not always observed.

Data set description i

- `Age`: the age of the patient (no missing values);
- `Lactate`: the conjugate base of lactic acid, upon arrival at the hospital (17.66% missing values);
- `Delta_hemo`: the difference between the hemoglobin upon arrival at hospital and the one in the ambulance (23.82% missing values);
- `VE`: binary variable indicating if a Volume Expander was applied in the ambulance. A volume expander is a type of intravenous therapy that has the function of providing volume for the circulatory system (2.46% missing values);
- `RBC`: a binary index which indicates whether the transfusion of Red Blood Cells Concentrates is performed (0.37% missing values);

Data set description ii

- `SI`: the shock index. It indicates the level of occult shock based on heart rate (HR) and systolic blood pressure (SBP), that is $\mathrm{SI} = \frac{\mathrm{HR}}{\mathrm{SBP}}$, upon arrival at hospital (2.09% missing values);
- `HR`: the heart rate measured upon arrival of hospital (1.62% missing values).

Results with CQR-MDA-Nested