Conformal prediction with missing values

Margaux Zaffran

LPSM PhD Students Seminar

February 20, 2023

Aymeric Dieuleveut
Ecole Polytechnique
Paris

Julie Josse
INRIA IDESP
Montpellier

Yaniv Romano
Technion - Israel Institute of Technology
Haifa

Motivation: critical medical care

TraumaBase®: decision support for trauma patients

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

TraumaBase®: decision support for trauma patients

- More than 30 000 trauma patients
- 30 hospitals
- 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.

TraumaBase®: decision support for trauma patients

- More than 30 000 trauma patients
- 30 hospitals
- 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.

Missing values: ubiquitous in data science pratice

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

Missing values: ubiquitous in data science pratice

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~~

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

Missing values: ubiquitous in data science pratice

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:

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

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

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

Missing values: ubiquitous in data science pratice

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:

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

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

One of the **ironies of Big Data** *is that missing data play an ever more significant role.*[1]

[1] 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**.

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

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

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

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

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

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

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

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

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

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

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

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

- Three **mechanisms**[2] can generate missing values.

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

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

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

- Three **mechanisms**[2] can generate missing values.
  $\hookrightarrow$ **Missing Completely At Random** (MCAR):
  $\mathbb{P}(M = m|X) = \mathbb{P}(M = m)$ for all $m \in \{0,1\}^d$.

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

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

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

- Three **mechanisms**[2] 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.

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

Supervised learning with missing values

Impute-then-regress procedures are widely used (Le Morvan et al., 2021).

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

Supervised learning with missing values

Impute-then-regress procedures are widely used (Le Morvan et al., 2021).

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

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

Supervised learning with missing values

Impute-then-regress procedures are widely used (Le Morvan et al., 2021).

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

$$
\begin{array}{c|c|c|c|c|}
x^{(1)} & -1 & -10 & 6 & 0 \\
x^{(2)} & 4 & \texttt{NA} & -2 & 2 \\
x^{(3)} & 5 & 1 & 2 & \texttt{NA} \\
x^{(4)} & 0 & \texttt{NA} & \texttt{NA} & 1
\end{array}
\xrightarrow{\quad \phi \quad}
\begin{array}{c|c|c|c|c|}
u^{(1)} & -1 & -10 & 6 & 0 \\
u^{(2)} & 4 & -4.5 & -2 & 2 \\
u^{(3)} & 5 & 1 & 2 & 1 \\
u^{(4)} & 0 & -4.5 & 3 & 1
\end{array}
$$

Supervised learning with missing values

Impute-then-regress procedures are widely used (Le Morvan et al., 2021).

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

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

Supervised learning with missing values

Impute-then-regress procedures are widely used (Le Morvan et al., 2021).

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

Le Morvan et al. (2021) show that for **any deterministic imputation** and **universal learner** this procedure is **Bayes-consistent**.

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

Back to predicting the levels of platelets

- **Challenging task:** Jiang et al. (2022) achieved an average relative prediction error ($\|\hat{y} - y\|^2/\|y\|^2$) no lower than 0.23

Back to predicting the levels of platelets

- **Challenging task:** Jiang et al. (2022) achieved an average relative prediction error ($\|\hat{y} - y\|^2 / \|y\|^2$) no lower than 0.23
- **Crucial task:** high-stakes decision-making problem

$\hookrightarrow$ High need for quantifying the predictive uncertainty.

Beyond point prediction?

Objective

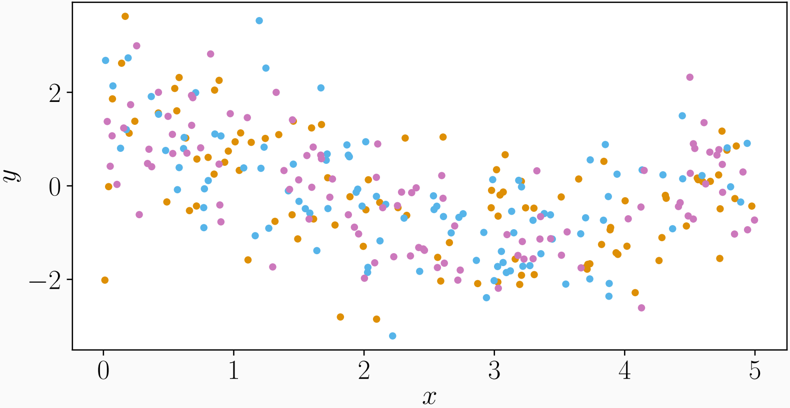
- Predict an unseen point $Y^{(n+1)}$ at $X^{(n+1)}$ with **confidence**
- Miscoverage level $\alpha \in [0, 1]$

▶ Build a predictive interval $\mathcal{C}_\alpha$ 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.

Split conformal prediction[1,2,3]: toy example

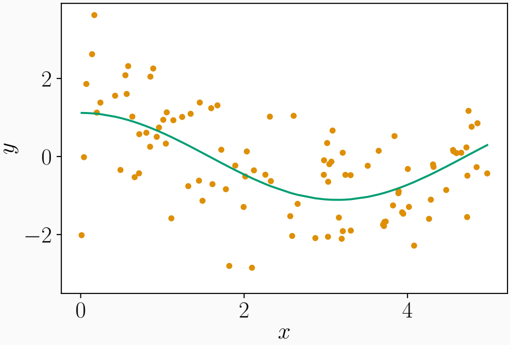


[1] Vovk et al. (2005), *Algorithmic Learning in a Random World*

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

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

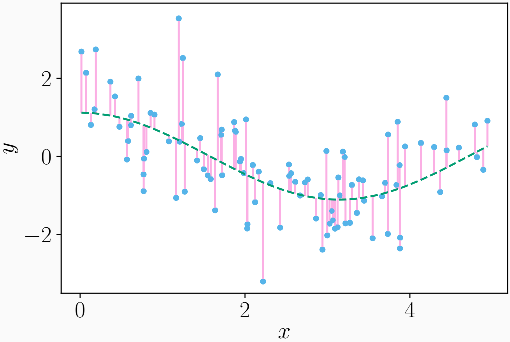
Split conformal prediction[1,2,3]: proper training step



- Learn $\hat{\mu}$

[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[1,2,3]: calibration step



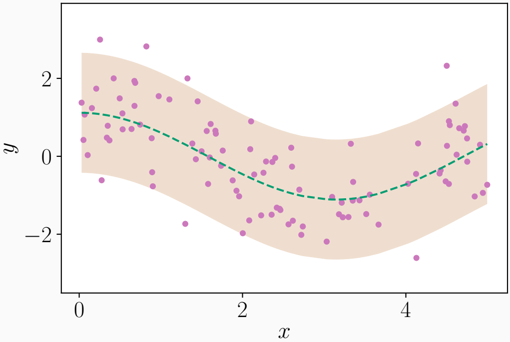
- Predict with $\hat{\mu}$
- Get the residuals $\hat{\varepsilon}^{(k)}$
- Compute the $(1-\alpha)\times(1+\frac{1}{\#\mathrm{Cal}})$ empirical quantile of the $|\hat{\varepsilon}^{(k)}|$, noted $Q_{1-\tilde{\alpha}}\left(|\hat{\varepsilon}^{(k)}|\right)$

[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[1,2,3]: prediction step



- Predict with $\hat{\mu}$
- Build $\widehat{C}_\alpha(x)$: $[\hat{\mu}(x) \pm Q_{1-\tilde{\alpha}}\left(|\hat{\varepsilon}^{(k)}|\right)]$

[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

Theory on SCP

Papadopoulos et al. (2002); Lei et al. (2018) prove that:

- given any regression function $\hat{\mu}$
- for any (**finite**) sample size n
- if the $(X^{(k)}, Y^{(k)})$ are **exchangeable**

then:

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

Theory on SCP

Papadopoulos et al. (2002); Lei et al. (2018) prove that:

- given any regression function $\hat{\mu}$
- for any (**finite**) sample size n
- if the $(X^{(k)}, Y^{(k)})$ are **exchangeable**

then:

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

If additionally the scores $\left|\hat{\varepsilon}_k\right|$ are almost surely distinct:

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

Split conformal prediction: summary

Split conformal prediction is simple to compute and works:

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

Split conformal prediction: summary

Split conformal prediction is simple to compute and works:

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

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

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

Split conformal prediction: summary

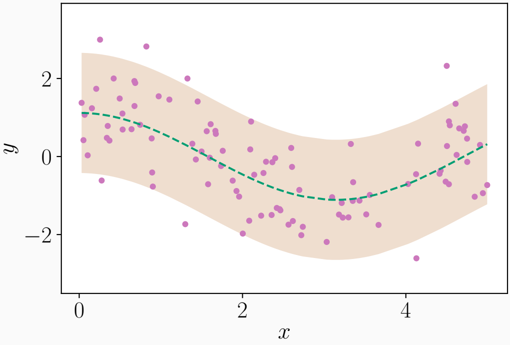
Split conformal prediction is simple to compute and works:

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

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

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

Split conformal prediction[1,2,3]: prediction step



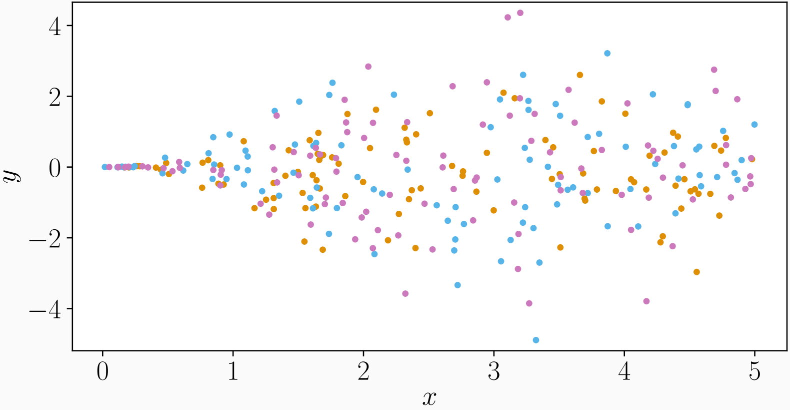
- Predict with $\hat{\mu}$
- Build $\widehat{C}_{\alpha}(x)$: $\left[\hat{\mu}(x) \pm Q_{1-\tilde{\alpha}}\left(\left|\hat{\varepsilon}^{(k)}\right|\right)\right]$

[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

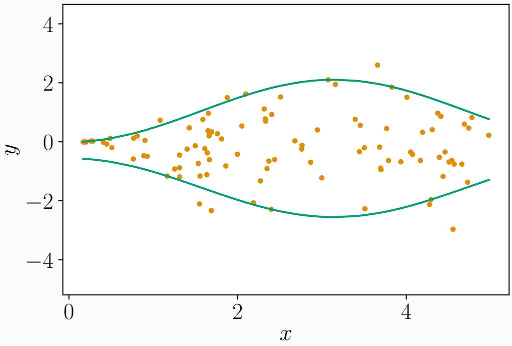
Conformalized Quantile Regression (Romano et al., 2019)



Randomly split the data to obtain a proper training set and a calibration set. Keep the test set.

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

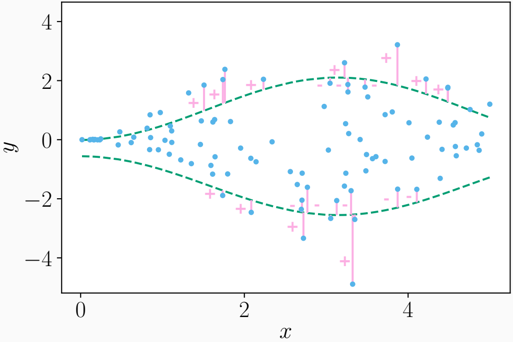
Conformalized Quantile Regression (Romano et al., 2019)



- Learn $\hat{q}_{\mathrm{inf}}$ and $\hat{q}_{\mathrm{sup}}$

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

Conformalized Quantile Regression (Romano et al., 2019)

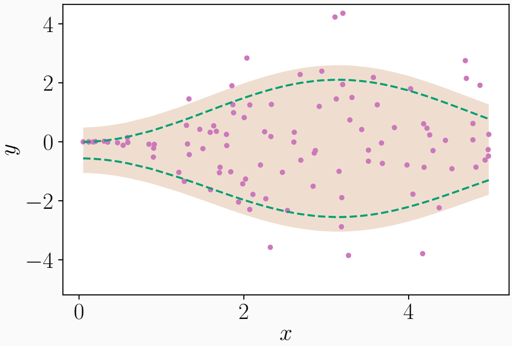


- Predict with $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- Get the scores $e^{(k)}$
- Compute the $(1-\alpha) \times (1 + \frac{1}{\#\text{Cal}})$ empirical quantile of the $e^{(k)}$, noted $Q_{1-\tilde{\alpha}}(e)$

$$\hookrightarrow \quad e^{(k)} := \max \left\{ \hat{q}_{\text{inf}}\left(x^{(k)}\right) - y^{(k)}, y^{(k)} - \hat{q}_{\text{sup}}\left(x^{(k)}\right) \right\}$$

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

Conformalized Quantile Regression (Romano et al., 2019)



- Predict with $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- Build $\hat{C}_\alpha(x)$:

$$\left[\hat{q}_{\text{inf}}(x) - Q_{1-\tilde{\alpha}}(e)\,,\; \hat{q}_{\text{sup}}(x) + Q_{1-\tilde{\alpha}}(e)\right]$$

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

Theory on CQR

Romano et al. (2019) prove that:

- given any quantile regression functions $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- for any (**finite**) sample size n
- if the $(X^{(k)}, Y^{(k)})$ are **exchangeable**

then:

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

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

Theory on CQR

Romano et al. (2019) prove that:

- given any quantile regression functions $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- for any (**finite**) sample size n
- if the $(X^{(k)}, Y^{(k)})$ are **exchangeable**

then:

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

If additionally the scores $e^{(k)}$ are almost surely distinct:

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

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

Conformal prediction with missing values

Impute-then-regress+conformalization is marginally valid

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

Impute-then-regress+conformalization is marginally valid

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

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

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

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

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

Impute-then-regress+conformalization is marginally valid

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

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

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

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

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

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

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

Impute-then-regress+conformalization is marginally valid

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

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

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

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

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

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

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

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

CQR performances on an illustrative example

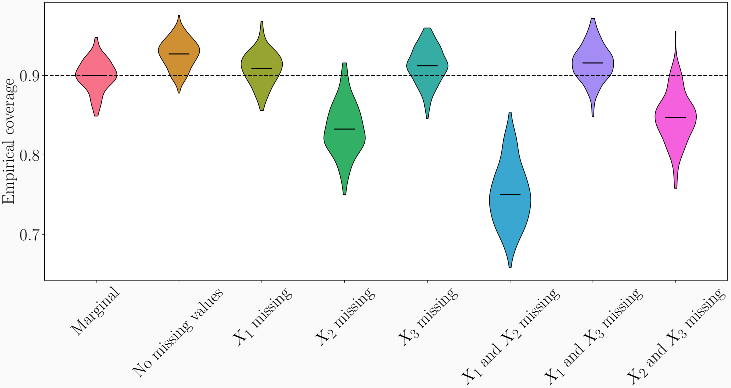
$$Y = \beta^T X + \varepsilon,$$

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

CQR performances on an illustrative example

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

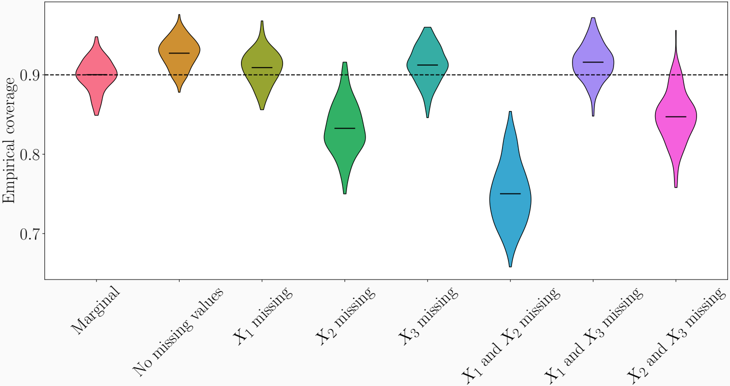
with $\beta = (1, 2, -1)^T$, $\varepsilon \perp\!\!\!\perp X$ and X and ε are Gaussian.



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**.

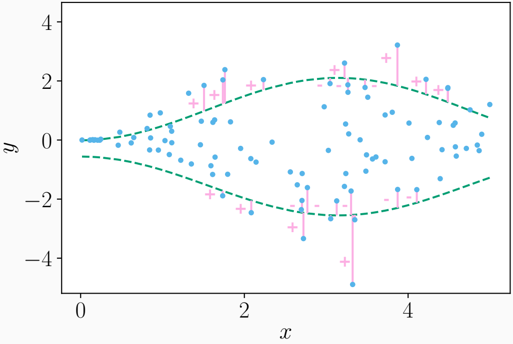
Missing data augmentation

Goal: validity conditionally to the mask

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

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

Issue during the calibration step



- Predict with $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- Get the scores $e^{(k)}$
- Compute the $(1-\alpha) \times (1 + \frac{1}{\#\mathrm{Cal}})$ empirical quantile of the $e^{(k)}$, noted $Q_{1-\tilde{\alpha}}(e)$

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

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

$$e^{(k)} = \max\left\{\hat{q}_{\mathrm{inf}}\left(\tilde{x}^{(k)}\right) - y^{(k)}, y^{(k)} - \hat{q}_{\mathrm{sup}}\left(\tilde{x}^{(k)}\right)\right\}$$

CQR-MDA with exact masking in words

1. Split your training set into a `proper training set` and `calibration set`
2. Train your imputation function on the `proper training set`
3. Impute the `proper training set`
4. Train your quantile regressors on the `imputed proper training set`
5. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:

CQR-MDA with exact masking in words

1. Split your training set into a `proper training set` and `calibration set`
2. Train your imputation function on the `proper training set`
3. Impute the `proper training set`
4. Train your quantile regressors on the `imputed proper training set`
5. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   5.1 For each $j \in [\![1, d]\!]$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \texttt{NA}$) for k in the `calibration set` such that $m^{(k)} \subset m^{(n+1)}$

CQR-MDA with exact masking in words

1. Split your training set into a `proper training set` and `calibration set`
2. Train your imputation function on the `proper training set`
3. Impute the `proper training set`
4. Train your quantile regressors on the `imputed proper training set`
5. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   5.1 For each $j \in [\![1, d]\!]$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \mathtt{NA}$) for k in the `calibration set` such that $m^{(k)} \subset m^{(n+1)}$
   5.2 Impute the `new calibration set`
   5.3 Compute the calibration correction
   5.4 Impute the test point
   5.5 Predict with the quantile regressors and the correction previously obtained

Conditional validity

Theorem (Zaffran et al., 2023)

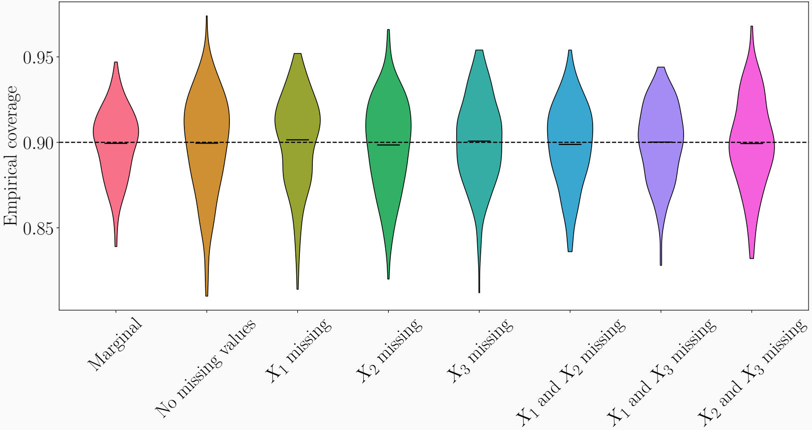
If the data is exchangeable and MCAR, then for almost all imputation function the proposed methodology is such that for any $m \in \mathcal{M} \subset \{0,1\}^d$:

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

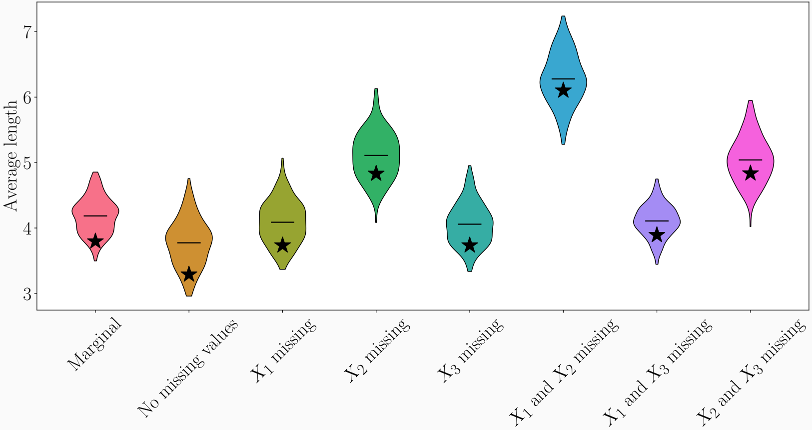
and if additionally the scores are almost surely distinct:

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

Empirical coverages

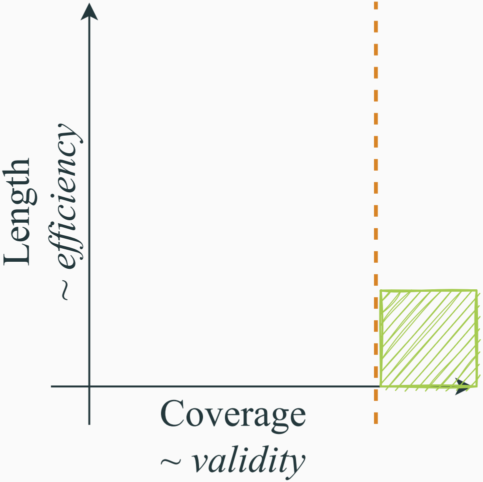


Empirical lengths

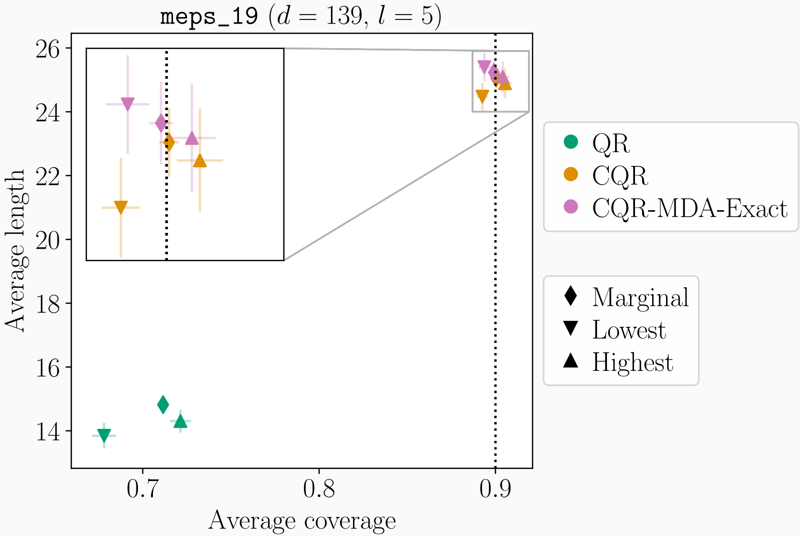


Experimental results

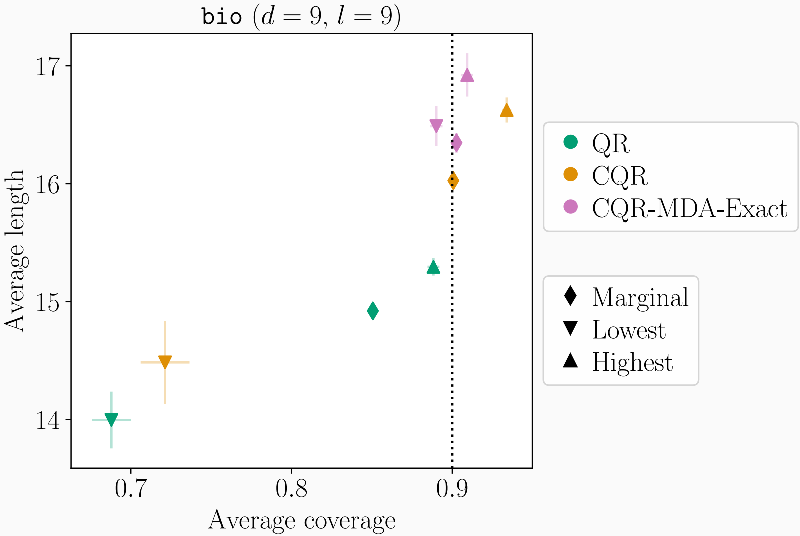
Visualisation



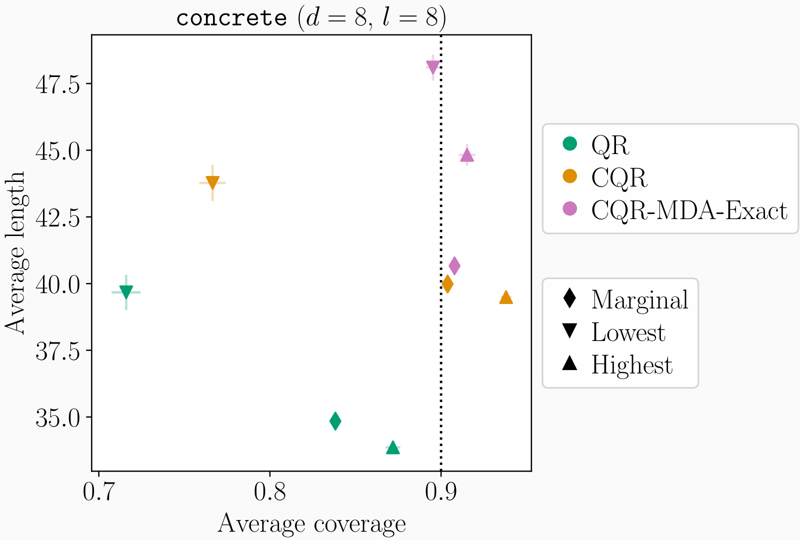
Semi-synthetic experiments



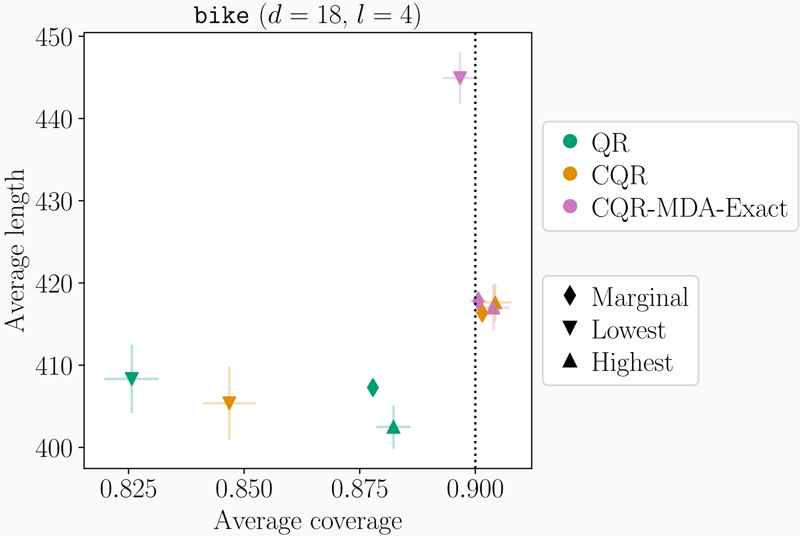
Semi-synthetic experiments

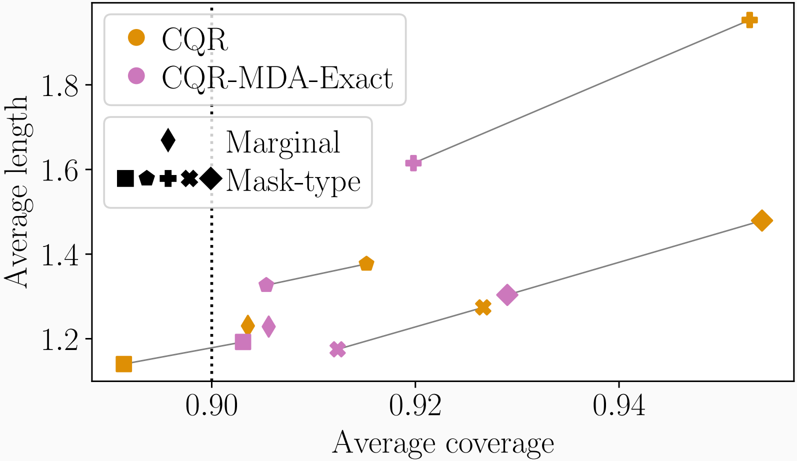


Semi-synthetic experiments



Semi-synthetic experiments




CQR
CQR-MDA-Exact
Marginal
Mask-type
1.8
1.6
1.4
1.2
Average length
0.90
0.92
0.94
Average coverage

Conclusion

Extensions

- Theoretical analysis of the Gaussian linear model ($Y = \beta^T X + \varepsilon$) corroborating our intuition.

Extensions

- Theoretical analysis of the Gaussian linear model ($Y = \beta^T X + \varepsilon$) corroborating our intuition.
- Consistency of universal quantile learner when chained with almost any imputation function.

Extensions

- Theoretical analysis of the Gaussian linear model ($Y = \beta^T X + \varepsilon$) corroborating our intuition.
- Consistency of universal quantile learner when chained with almost any imputation function.
- CP-MDA-Nested, an algorithm which does not discard any calibration point.

Take-home-messages

- CP marginal guarantees hold on the imputed data set.

Take-home-messages

- CP marginal guarantees hold on the imputed data set.
- Missingness introduces additional heteroskedasticity, creating a need for quantile regression based methods.

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.

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**.

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!

Jiang, W., Bogdan, M., Josse, J., Majewski, S., Miasojedow, B., Ročková, V., and TraumaBase® Group (2022). Adaptive bayesian slope: Model selection with incomplete data. *Journal of Computational and Graphical Statistics*, 31(1):113–137.

Le Morvan, M., Josse, J., Scornet, E., and Varoquaux, G. (2021). What's a good imputation to predict with missing values? *NeurIPS*.

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*.

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

Romano, Y., Patterson, E., and Candès, E. (2019). Conformalized Quantile Regression. *NeurIPS*.

Rubin, D. B. (1976). Inference and missing data. *Biometrika*, 63(3):581–592.

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

Zhu, Z., Wang, T., and Samworth, R. J. (2019). High-dimensional principal component analysis with heterogeneous missingness.

Gaussian linear model

Missing values induce heteroskedasticity

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

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.)

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

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

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.)

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

- 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)

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)
- The uncertainty increases when there are more missing values

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

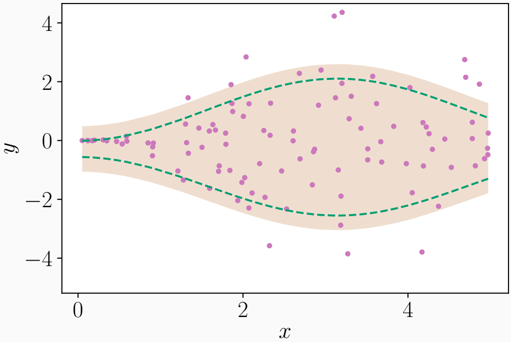
Initial calibration set

$x^{(1)}$	-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

What if we kept all individuals?



- Predict with $\hat{q}_{\text{inf}}$ and $\hat{q}_{\text{sup}}$
- Build $\hat{C}_{\hat{\alpha}}(x)$:

$$\left[\hat{q}_{\text{inf}}(x) - Q_{1-\tilde{\alpha}}(e), \; \hat{q}_{\text{sup}}(x) + Q_{1-\tilde{\alpha}}(e)\right]$$

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 $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   1.1 For each $j \in [\![1, d]\!]$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \texttt{NA}$) for k in the `calibration set` such that $m^{(k)} \subset m^{(n+1)}$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
    1.1 For each $j \in [\![1, d]\!]$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \texttt{NA}$) for k in the `calibration set`

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   1.1 Set $\tilde{m}^{(k)} = \max(m^{(k)}, m^{(n+1)})$ for k in the `calibration set`

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   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`

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
    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:

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   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 $e^{(k)}$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
    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 $e^{(k)}$
        1.3.2 Impute-then-predict on the augmented test point $(x^{(n+1)}, \tilde{m}^{(k)})$, giving: $\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k})$ and $\hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k})$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
    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 $e^{(k)}$
        1.3.2 Impute-then-predict on the augmented test point $(x^{(n+1)}, \tilde{m}^{(k)})$, giving: $\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k})$ and $\hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k})$
        1.3.3 Compute the corrected prediction interval: $[\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k}) - e^{(k)}; \hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k}) + e^{(k)}] := \left[z_{\text{inf}}^{(k)}; z_{\text{sup}}^{(k)}\right]$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   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 $e^{(k)}$
      1.3.2 Impute-then-predict on the augmented test point $(x^{(n+1)}, \tilde{m}^{(k)})$, giving: $\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k})$ and $\hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k})$
      1.3.3 Compute the corrected prediction interval: $[\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k}) - e^{(k)}; \hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k}) + e^{(k)}] := \left[z_{\text{inf}}^{(k)}; z_{\text{sup}}^{(k)}\right]$
   1.4 Compute the quantiles $Q_{\tilde{\alpha}}(\{z_{\text{inf}}^{(k)}\}_{k\in\mathrm{Cal}})$ and $Q_{1-\tilde{\alpha}}(\{z_{\text{sup}}^{(k)}\}_{k\in\mathrm{Cal}})$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
   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 $e^{(k)}$
      1.3.2 Impute-then-predict on the augmented test point $(x^{(n+1)}, \tilde{m}^{(k)})$, giving: $\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k})$ and $\hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k})$
      1.3.3 Compute the corrected prediction interval: $[\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k}) - e^{(k)}; \hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k}) + e^{(k)}] := \left[z_{\text{inf}}^{(k)}; z_{\text{sup}}^{(k)}\right]$
   1.4 Compute the quantiles $Q_{\tilde{\alpha}}(\{z_{\text{inf}}^{(k)}\}_{k\in\mathrm{Cal}})$ and $Q_{1-\tilde{\alpha}}(\{z_{\text{sup}}^{(k)}\}_{k\in\mathrm{Cal}})$
   1.5 Predict $[Q_{\tilde{\alpha}}(\{z_{\text{inf}}^{(k)}\}_{k\in\mathrm{Cal}}); Q_{1-\tilde{\alpha}}(\{z_{\text{sup}}^{(k)}\}_{k\in\mathrm{Cal}})]$

CQR-MDA with nested masking in words

1. For a test point $\left(x^{(n+1)}, m^{(n+1)}\right)$:
    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 $e^{(k)}$
        1.3.2 Impute-then-predict on the augmented test point $(x^{(n+1)}, \tilde{m}^{(k)})$, giving: $\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k})$ and $\hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k})$
        1.3.3 Compute the corrected prediction interval: $[\hat{q}_{\text{inf}}(\tilde{x}^{(n+1),k}) - e^{(k)}; \hat{q}_{\text{sup}}(\tilde{x}^{(n+1),k}) + e^{(k)}] := \left[z_{\text{inf}}^{(k)}; z_{\text{sup}}^{(k)}\right]$
    1.4 Compute the quantiles $Q_{\tilde{\alpha}}(\{z_{\text{inf}}^{(k)}\}_{k\in\mathrm{Cal}})$ and $Q_{1-\tilde{\alpha}}(\{z_{\text{sup}}^{(k)}\}_{k\in\mathrm{Cal}})$
    1.5 Predict $[Q_{\tilde{\alpha}}(\{z_{\text{inf}}^{(k)}\}_{k\in\mathrm{Cal}}); Q_{1-\tilde{\alpha}}(\{z_{\text{sup}}^{(k)}\}_{k\in\mathrm{Cal}})]$

Summary of CP-MDA

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

CP-MDA with exact masking:

calibration set

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

CP-MDA with nested masking:

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

and

temporary test points

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

Towards asymptotic individualized coverage

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

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

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

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

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

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

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

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

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.

Settings of the experiments

Some settings

- Imputation by iterative ridge ($\sim$ conditional expectation)

Some settings

- Imputation by iterative ridge ($\sim$ conditional expectation)
- **Concatenate the mask in the features**

Some settings

- Imputation by iterative ridge ($\sim$ conditional expectation)
- **Concatenate the mask in the features**
- Neural network, fitted to minimize the pinball loss

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:

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%

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

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
  - Various test sets

$$d = 3$$

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

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

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

Data generation

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

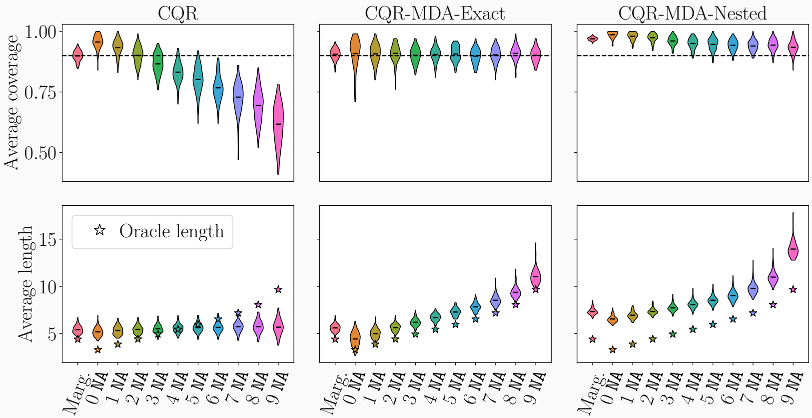
$Y = \beta X + \varepsilon$

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

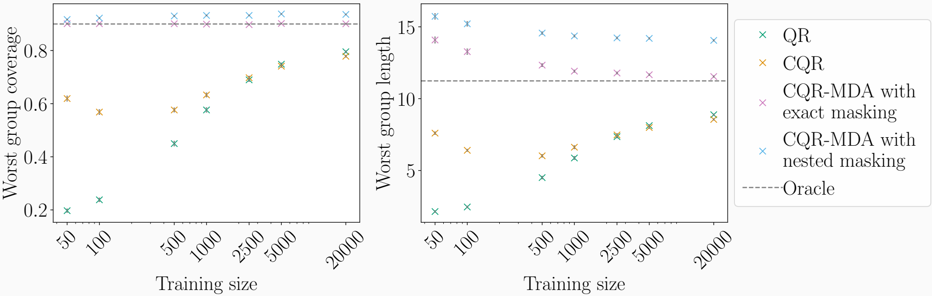
and $(X_1, \cdots, X_{10}) \sim \mathcal{N}\left(\begin{pmatrix} 1 \\ \vdots \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} 1 & 0.8 & \cdots & 0.8 \\ 0.8 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0.8 \\ 0.8 & \cdots & 0.8 & 1 \end{pmatrix}\right)$.

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

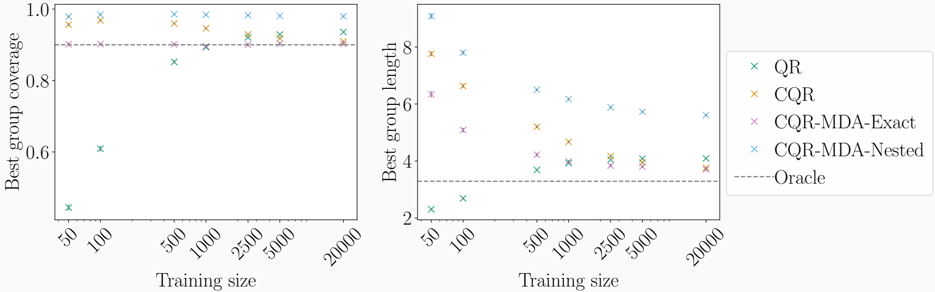
Synthetic experiments (Gaussian linear model, $d = 10$)



Results on the worst group

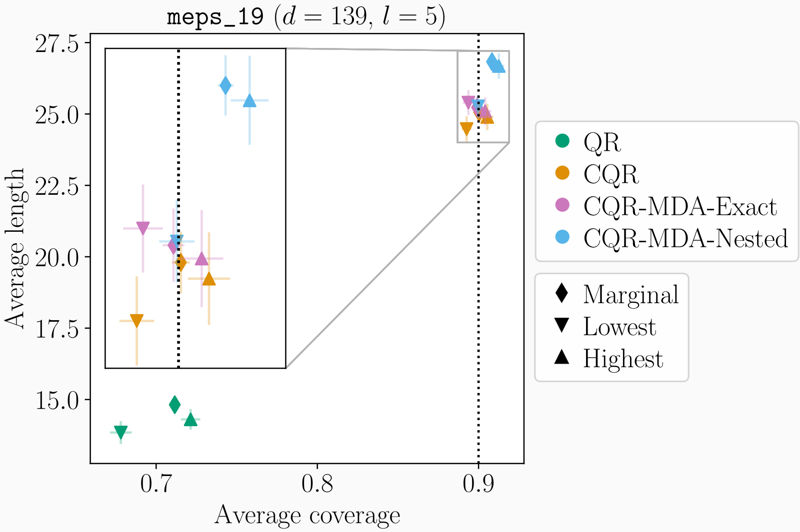


Results on the best group

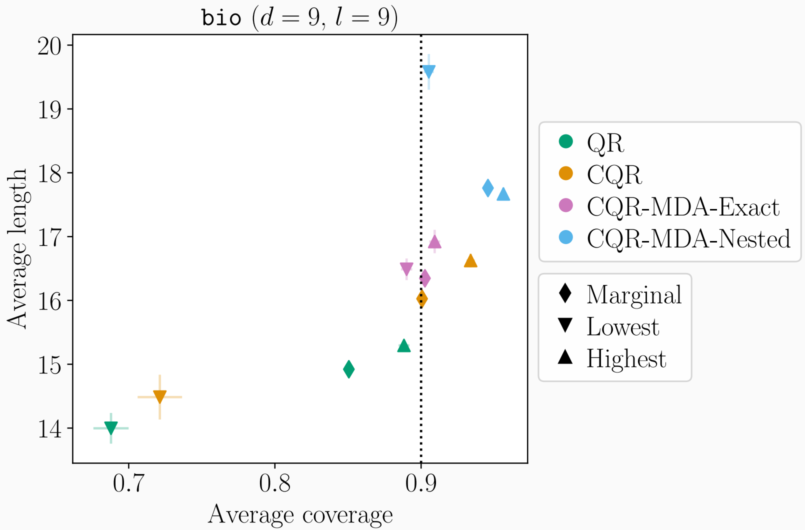


Semi-synthetic experiments with CQR-MDA-Nested

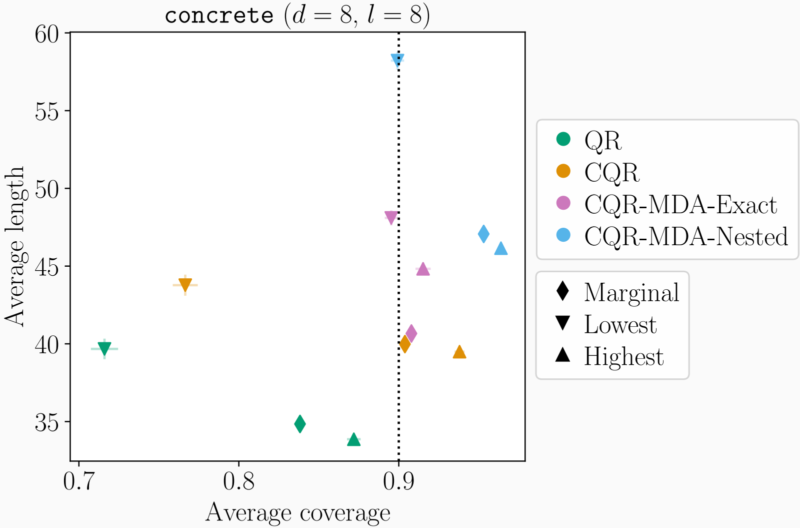
Semi-synthetic experiments with the CQR-MDA-Nested



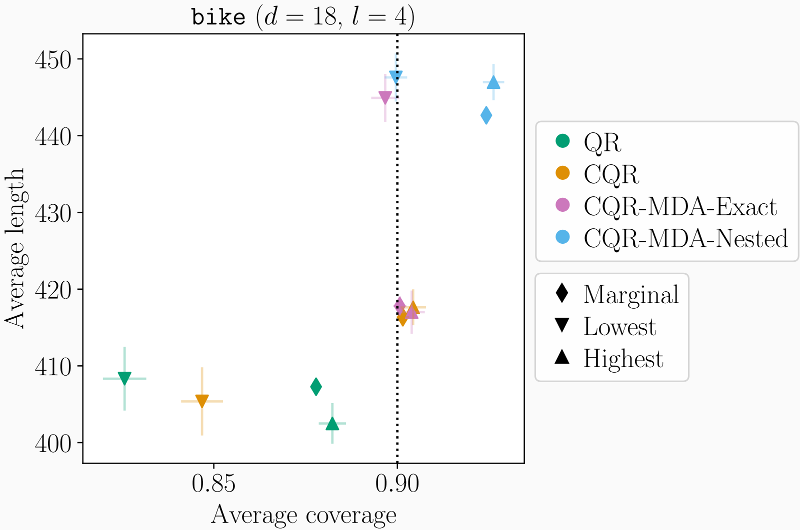
Semi-synthetic experiments with the CQR-MDA-Nested



Semi-synthetic experiments with the CQR-MDA-Nested



Semi-synthetic experiments with the CQR-MDA-Nested



TraumaBase

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