

Conformal prediction with missing values

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Causal Inference and Missing Data Seminar, INRIA

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Motivation: critical medical care

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
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These covariates are not always observed.

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

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

¹Zhu 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.
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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

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

ϕ

$u^{(1)}$	-1	-10	6	0
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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: $\left\{ \underbrace{\phi\left(x_{\text{obs}(m^{(k)})}^{(k)}, m^{(k)}\right)}_{\text{imputed } x^{(k)}}, y^{(k)} \right\}_{k=1}^n$.

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

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

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- **Crucial task:** high-stakes decision-making problem

↔ High need for **quantifying** the **predictive uncertainty**.

Beyond point prediction?

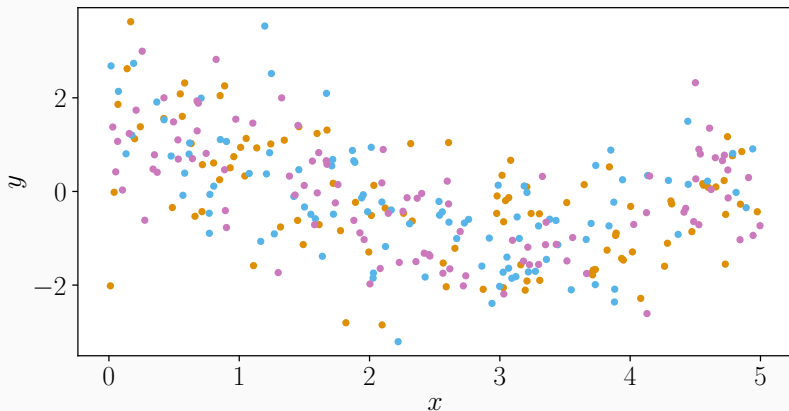
Objective

- 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}_α such that:

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

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

Split conformal prediction^{1,2,3}: toy example

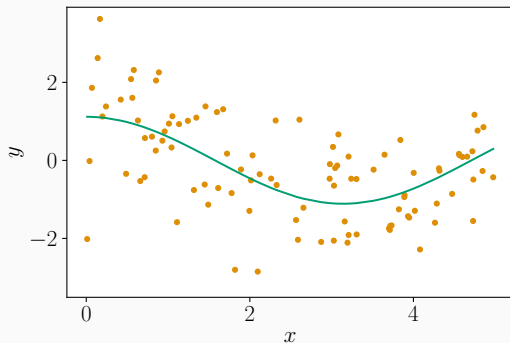


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Split conformal prediction^{1,2,3}: proper training step



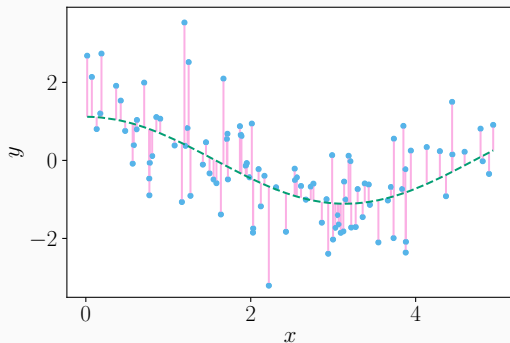
► Learn $\hat{\mu}$

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Split conformal prediction^{1,2,3}: calibration step



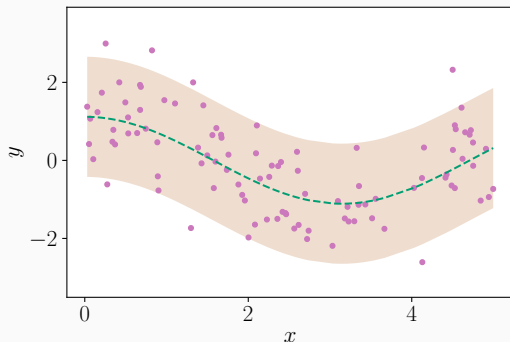
- ▶ Predict with $\hat{\mu}$
- ▶ Get the residuals $\hat{\epsilon}^{(k)}$
- ▶ Compute the $(1 - \alpha) \times (1 + \frac{1}{\#\text{Cal}})$ empirical quantile of the $|\hat{\epsilon}^{(k)}|$, noted $Q_{1-\tilde{\alpha}}(|\hat{\epsilon}^{(k)}|)$

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Split conformal prediction^{1,2,3}: prediction step



► Predict with $\hat{\mu}$

► Build $\hat{C}_\alpha(x)$:

$$[\hat{\mu}(x) \pm Q_{1-\tilde{\alpha}}(|\hat{\varepsilon}^{(k)}|)]$$

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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:

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If additionally the scores $|\hat{\epsilon}^{(k)}|$ are almost surely distinct:

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Split conformal prediction: summary

Split conformal prediction is simple to compute and works:

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

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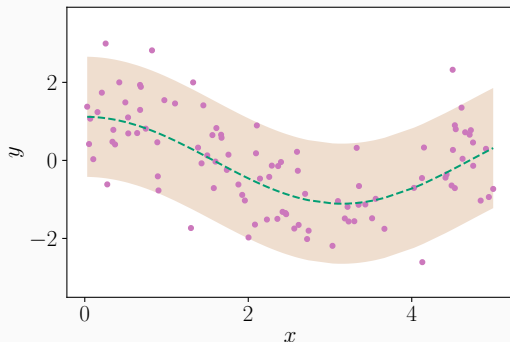
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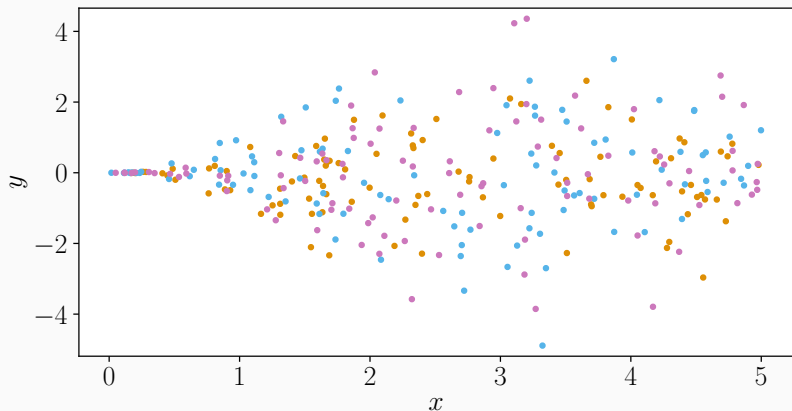
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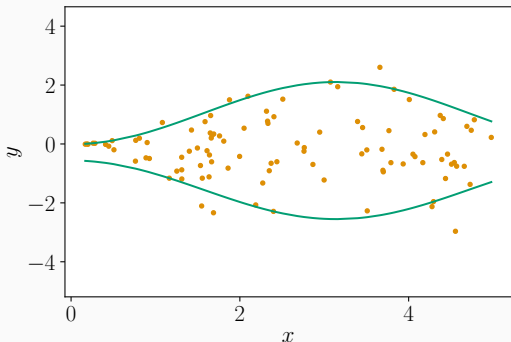
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Conformalized Quantile Regression (Romano et al., 2019)



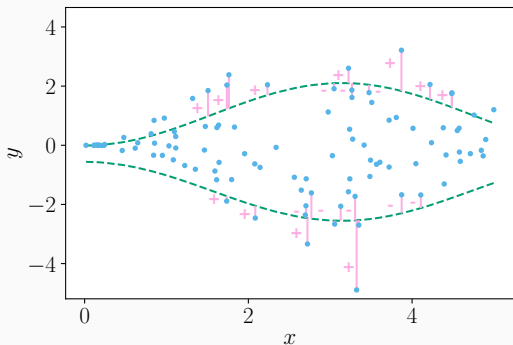
Randomly split the data to obtain a **proper training set** and a **calibration set**. Keep the **test set**.

Conformalized Quantile Regression (Romano et al., 2019)



► Learn \hat{q}_{inf} and \hat{q}_{sup}

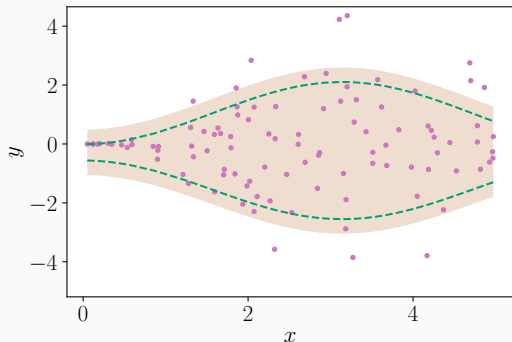
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- ▶ Predict with \hat{q}_{inf} and \hat{q}_{sup}
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- ▶ Compute the $(1 - \alpha) \times (1 + \frac{1}{\#\text{Cal}})$ empirical quantile of the $e^{(k)}$, noted $Q_{1-\tilde{\alpha}}(e)$

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

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

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

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\Rightarrow Conformal prediction applied on an imputed data set still enjoys marginal guarantees³:

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

³The upper bound also holds under continuously distributed scores.

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

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CQR performances on an illustrative example

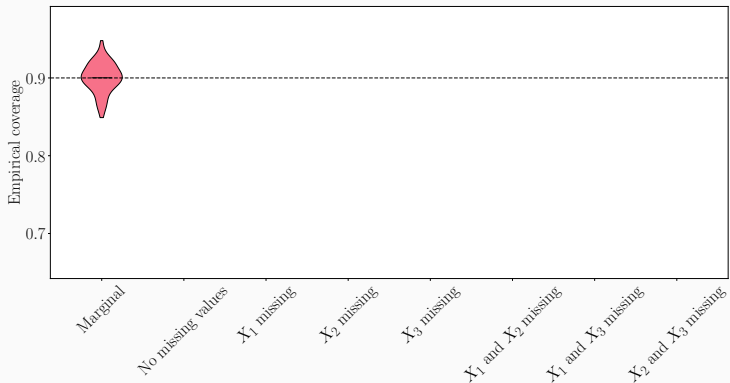
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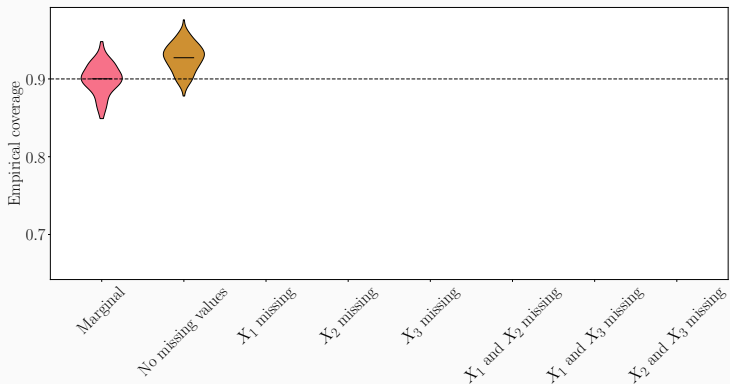
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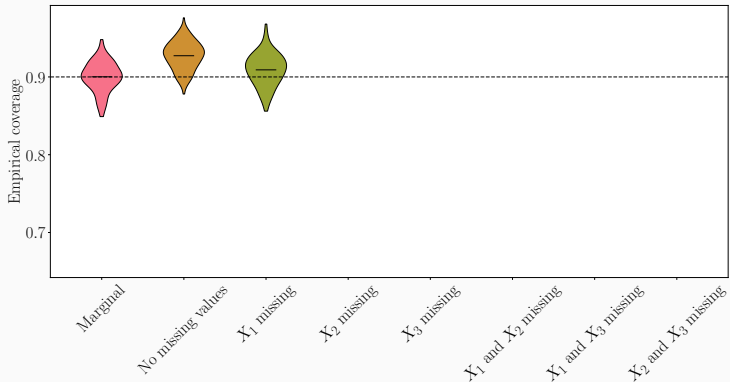
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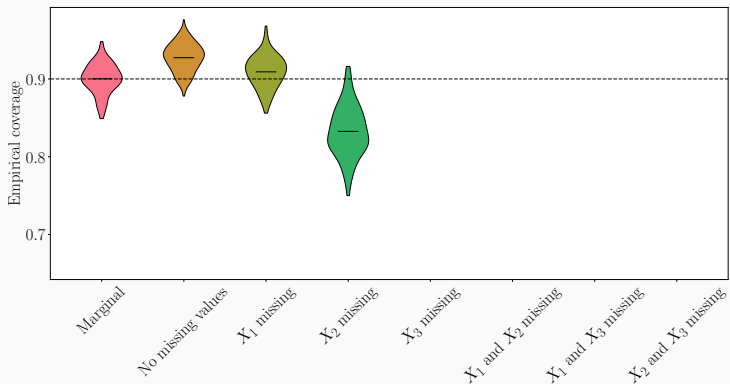
with $\beta = (1, 2, -1)^T$, $\varepsilon \perp\!\!\!\perp X$ and X and ε are Gaussian.



CQR performances on an illustrative example

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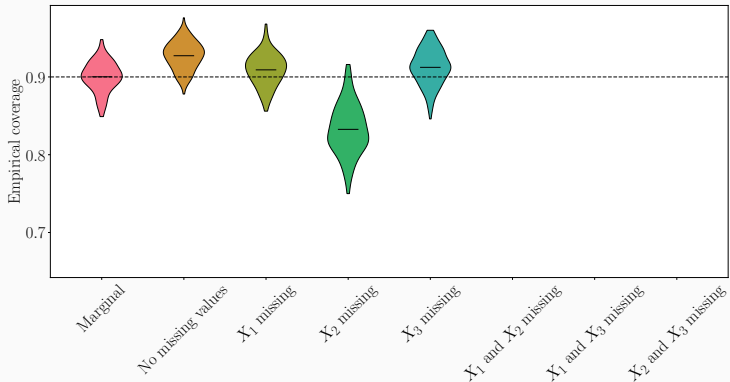
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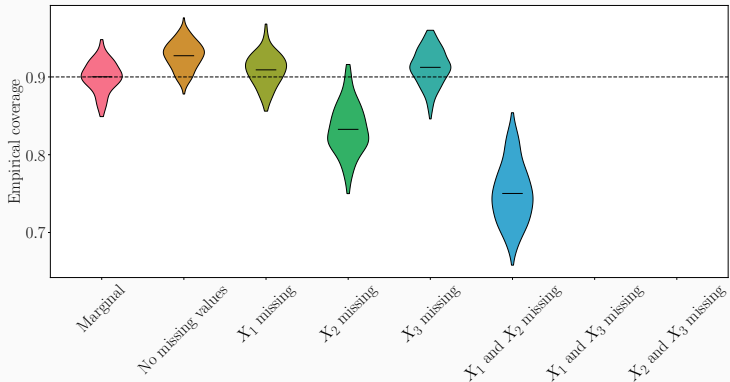
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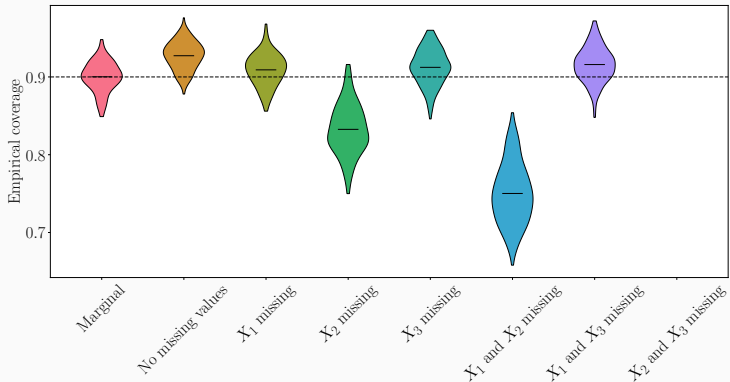
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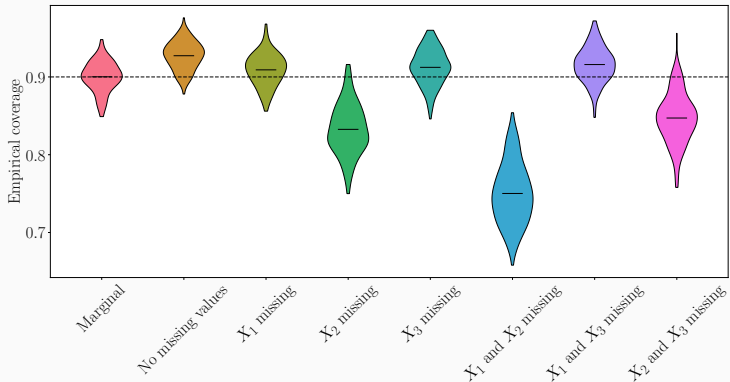
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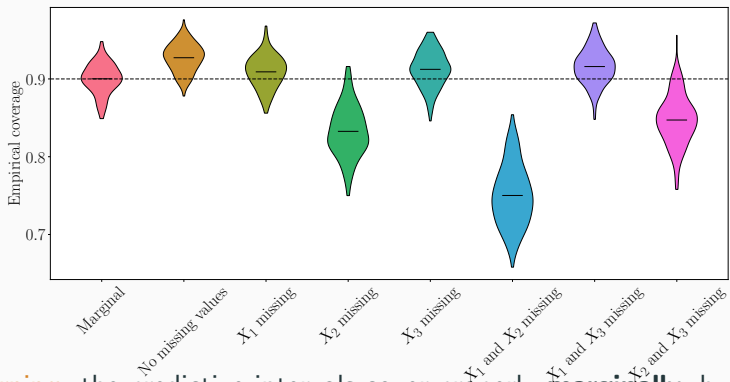
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with $\beta = (1, 2, -1)^T$, $\varepsilon \perp\!\!\!\perp X$ and X and ε are Gaussian.



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:

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- 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)

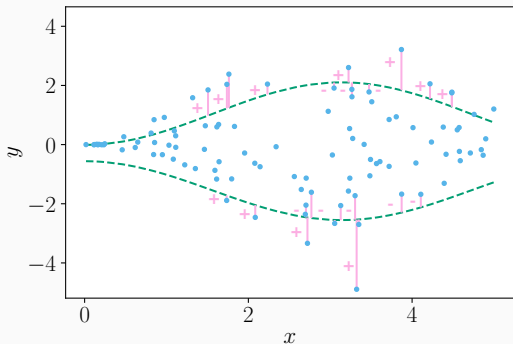
Missing data augmentation

Goal: validity conditionally to the mask

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

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

Issue during the calibration step



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

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
$\tilde{x}^{(3)}$	[Hatched area]			
$\tilde{x}^{(4)}$	0	NA	NA	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 $(x^{(n+1)}, m^{(n+1)})$:

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 - 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

Theorem (Zaffran et al., 2023)

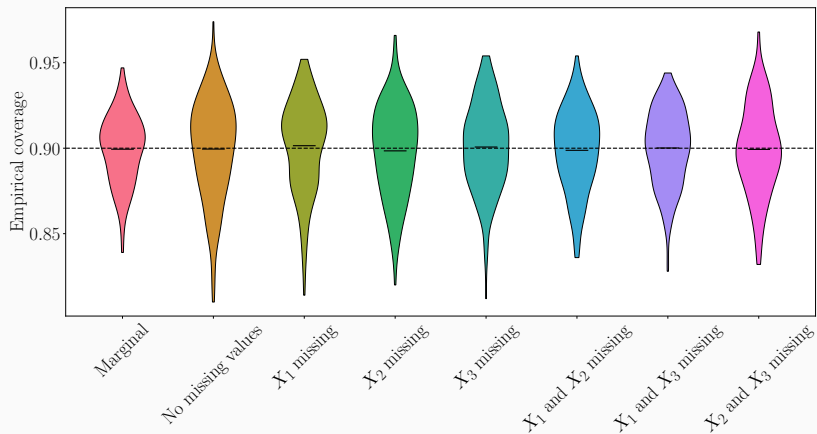
If the data is exchangeable and MCAR, then for almost all imputation function the proposed methodology is such that for any $m \in \mathcal{M} \subset \{0, 1\}^d$:

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

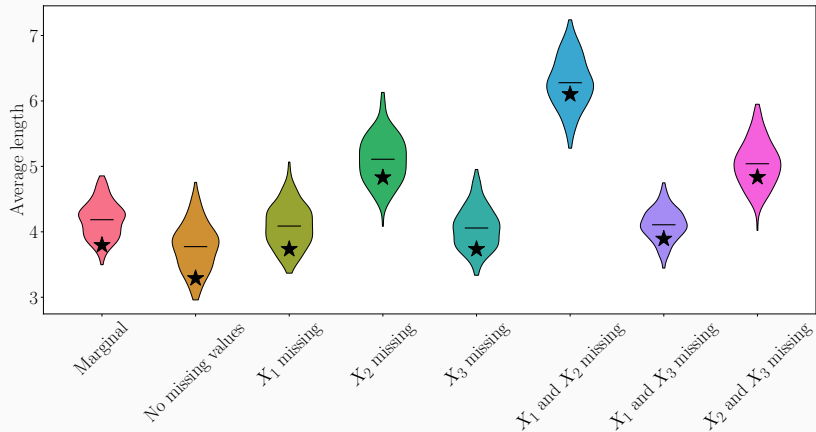
and if additionally the scores are almost surely distinct:

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

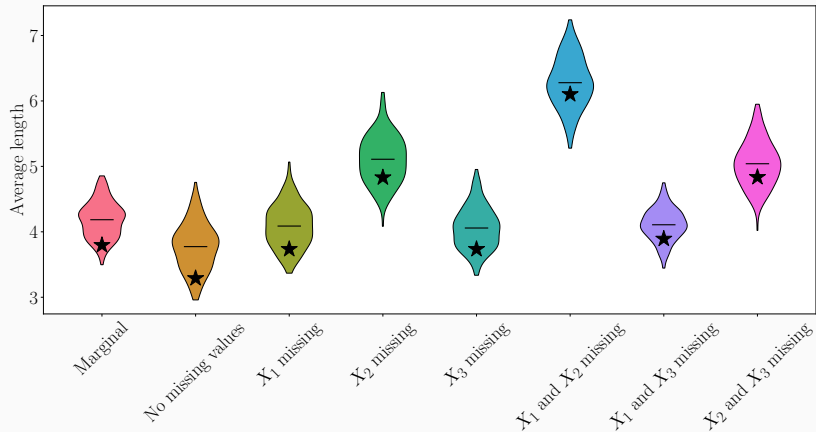
Empirical coverages



Empirical lengths



Empirical lengths



[link to CP-MDA-Nested](#)

Experimental results

- Imputation by iterative ridge (\sim conditional expectation)

Some settings

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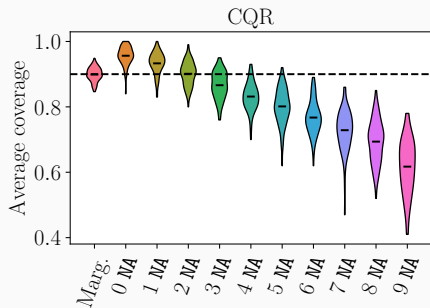
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 - MCAR missing values, with probability 20%

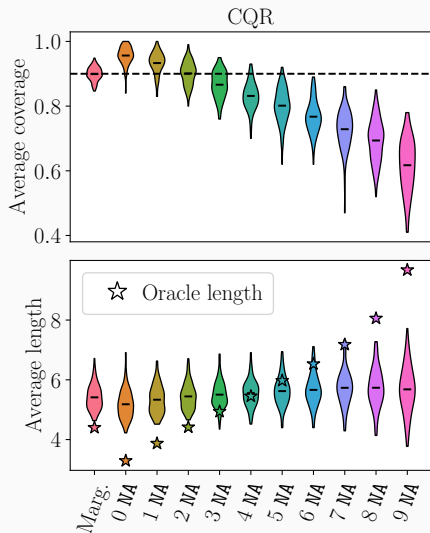
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- (Semi)-synthetic experiments:
 - MCAR missing values, with probability 20%
 - 100 repetitions
 - Various test sets

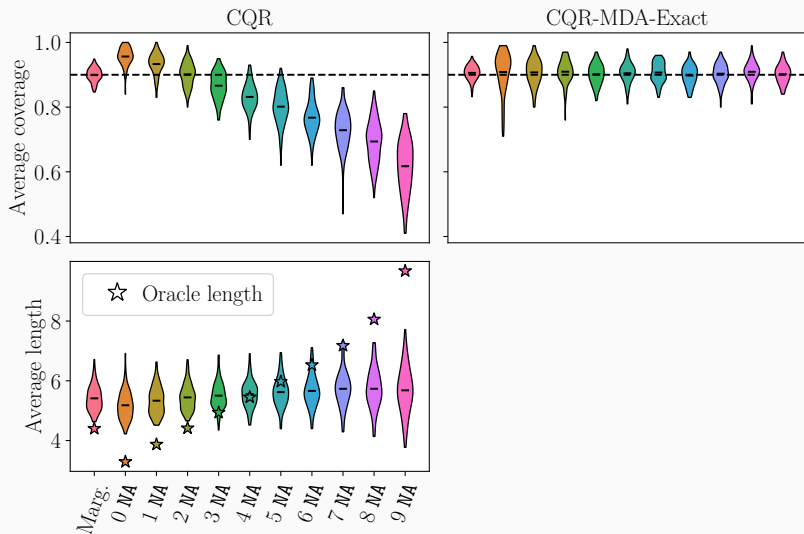
Synthetic experiments (Gaussian linear model, $d = 10$)



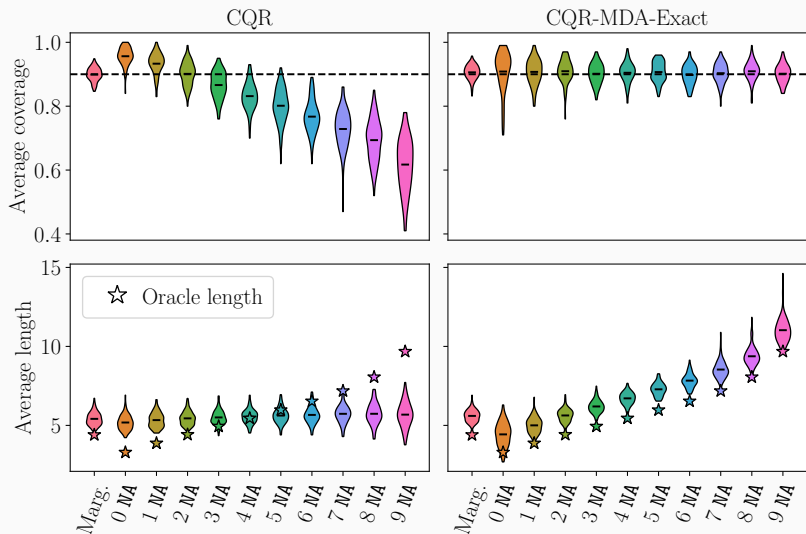
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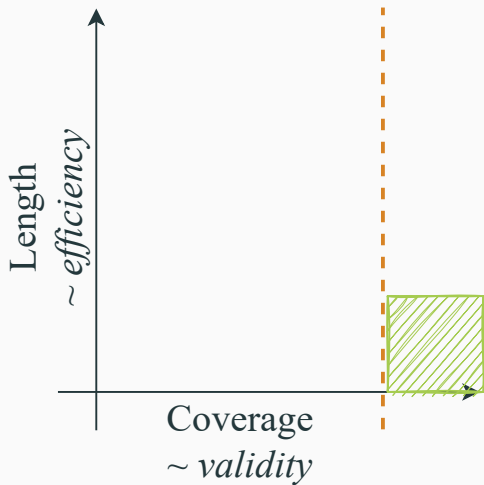
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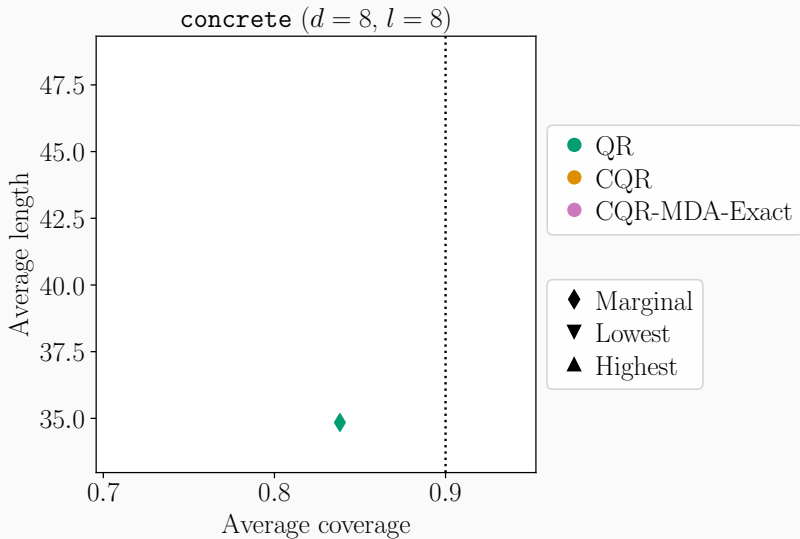
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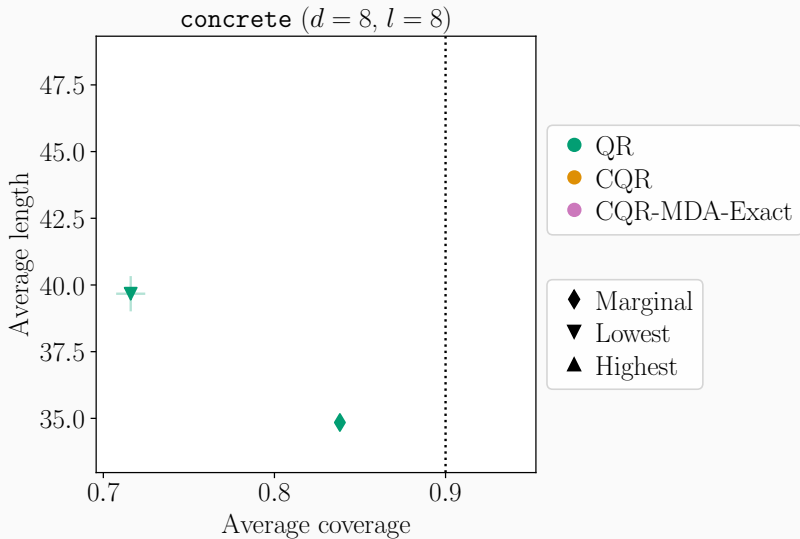
Before more experiments, visualisation



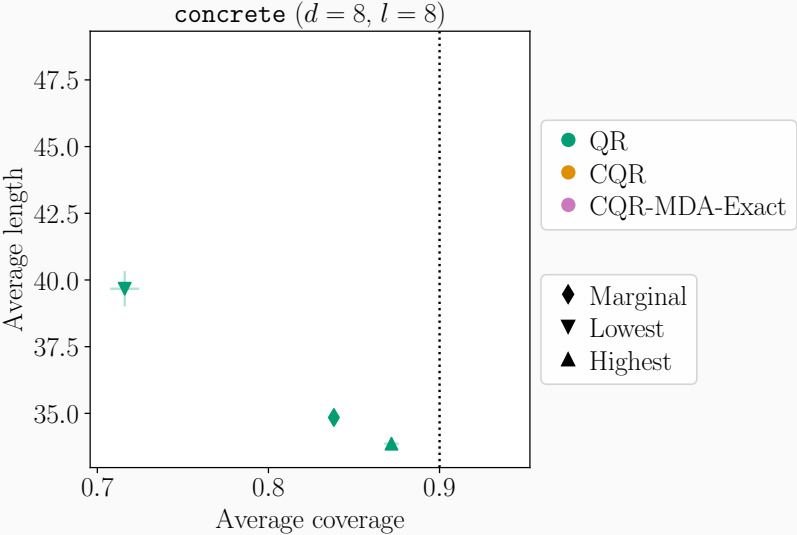
Semi-synthetic experiments



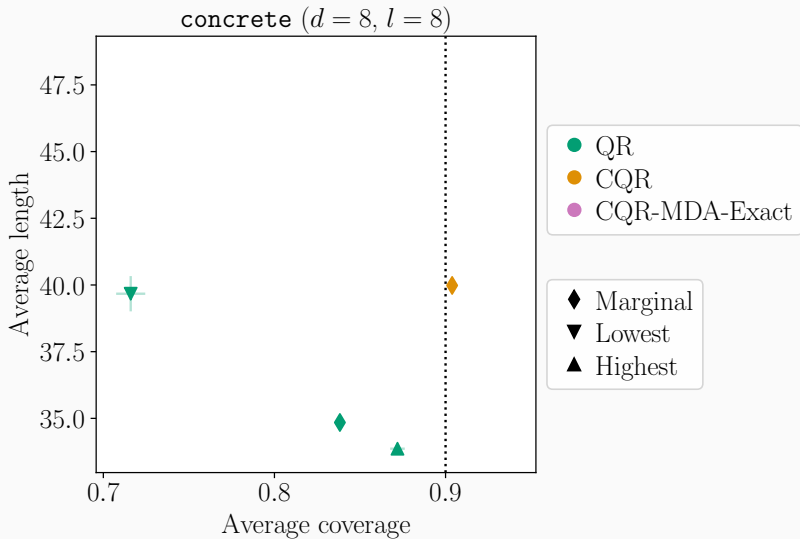
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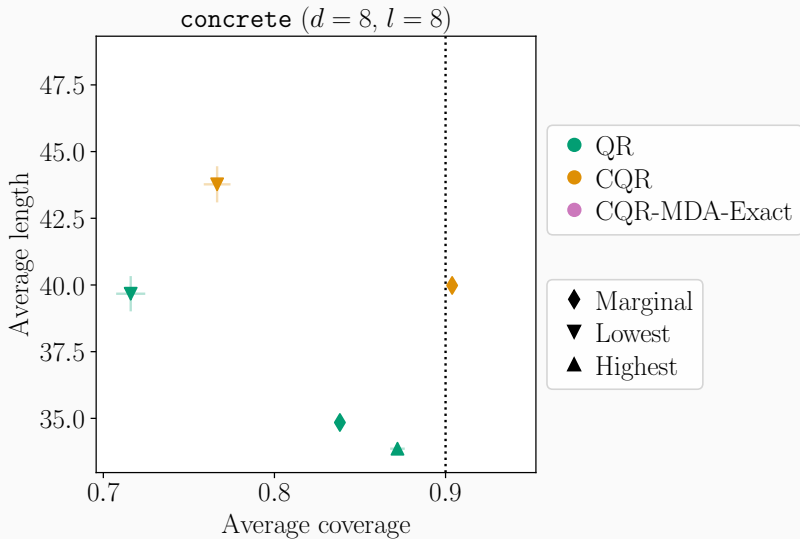
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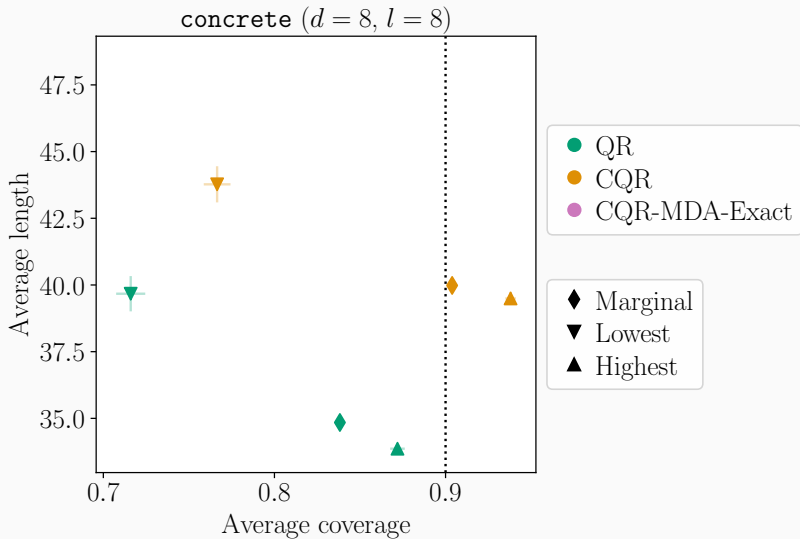
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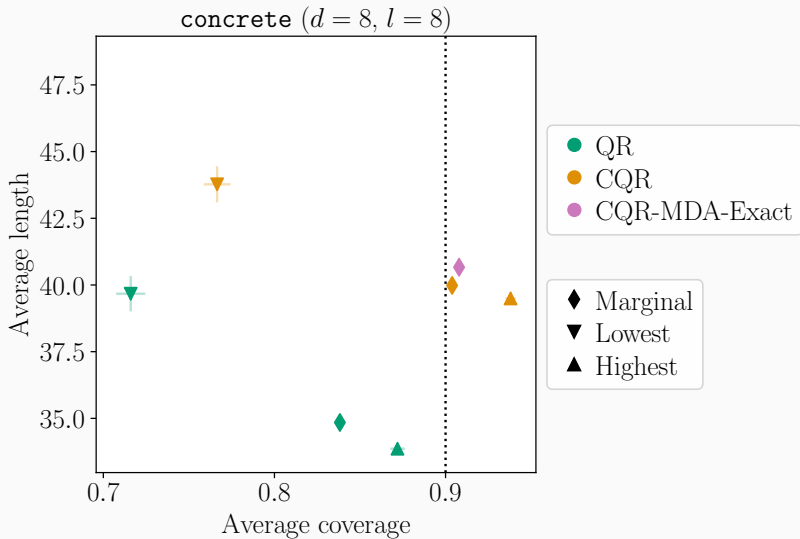
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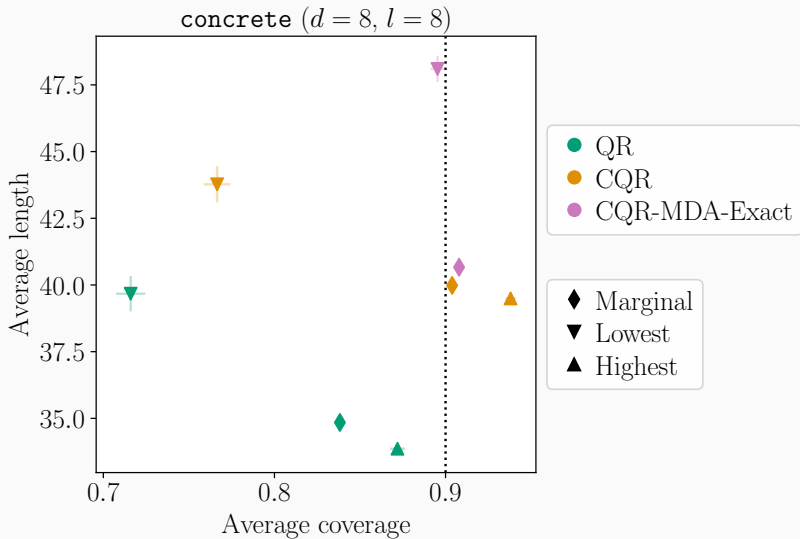
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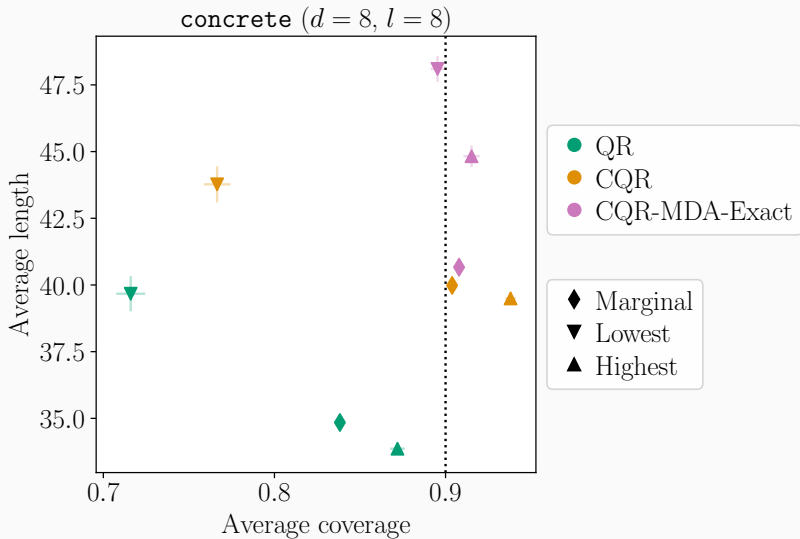
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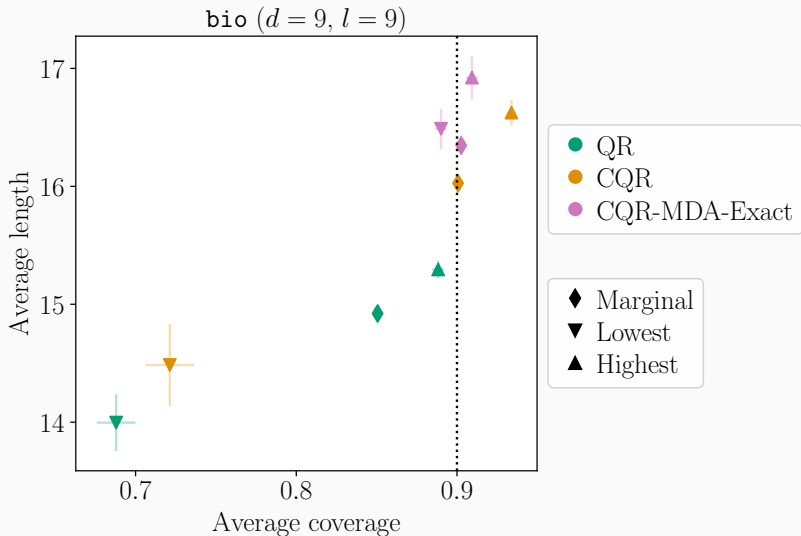
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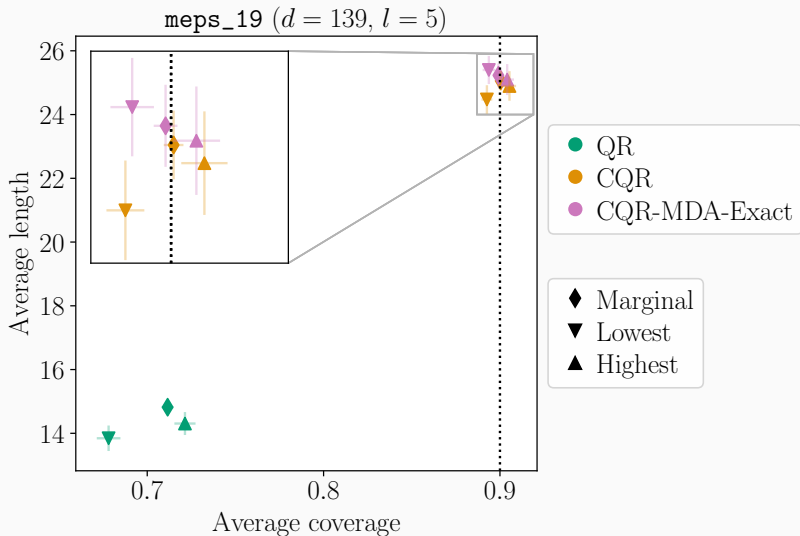
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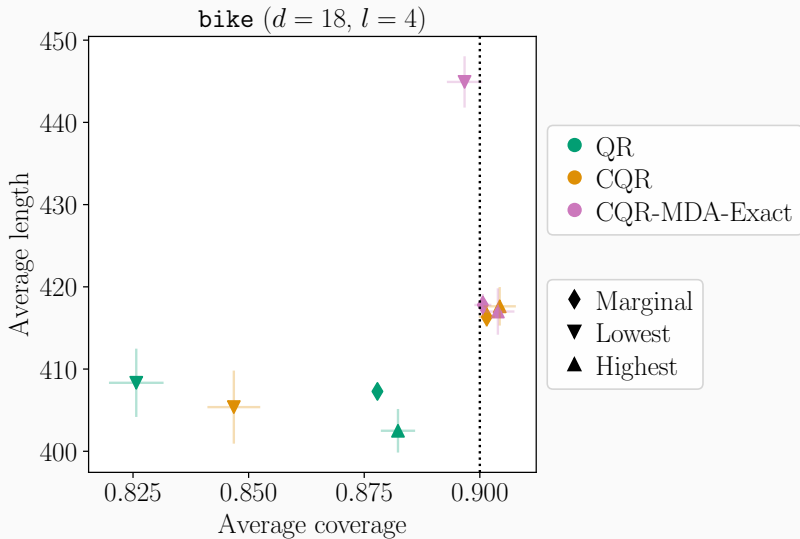
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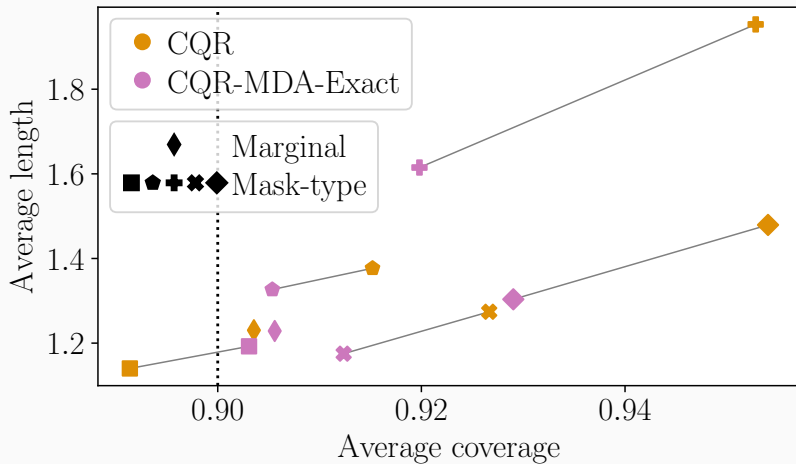
Semi-synthetic experiments



Semi-synthetic experiments



Real data experiment: back to critical care medicine



Conclusion

- Consistency of universal quantile learner when chained with almost any imputation function.

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- CP-MDA-Nested, an algorithm which does not discard any calibration point.

- CP marginal guarantees hold on the imputed data set.

Take-home-messages

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- **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).

Long version: 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
$\tilde{x}^{(3)}$	[Hatched area]			
$\tilde{x}^{(4)}$	0	NA	NA	1

What if we kept all individuals?

Test point

3	NA	NA	1
---	----	----	---

Initial calibration set

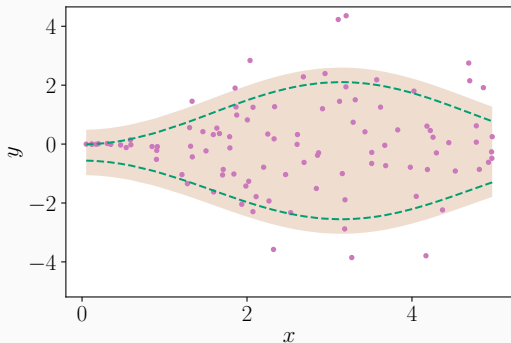
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What if we kept all individuals?



► Predict with \hat{q}_{inf} and \hat{q}_{sup}

► Build $\hat{C}_{\hat{\alpha}}(x)$:

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

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
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Calibration set used

$\tilde{x}^{(1)}$	-1	NA	NA	1
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Temporary test points

and

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 $(x^{(n+1)}, m^{(n+1)})$:
 - 1.1 For each $j \in \llbracket 1, d \rrbracket$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \text{NA}$) for k in the calibration set **such that**
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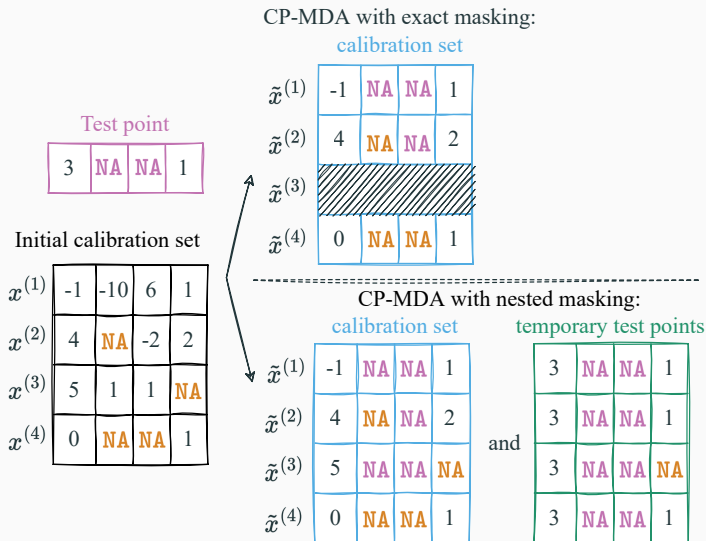
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Summary of CP-MDA



Experimental results

- 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

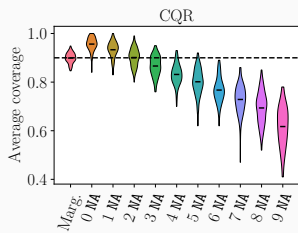
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 - MCAR missing values, with probability 20%

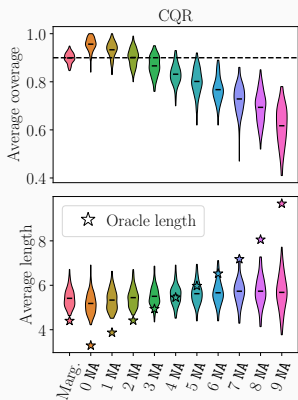
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- (Semi)-synthetic experiments:
 - MCAR missing values, with probability 20%
 - 100 repetitions
 - Various test sets

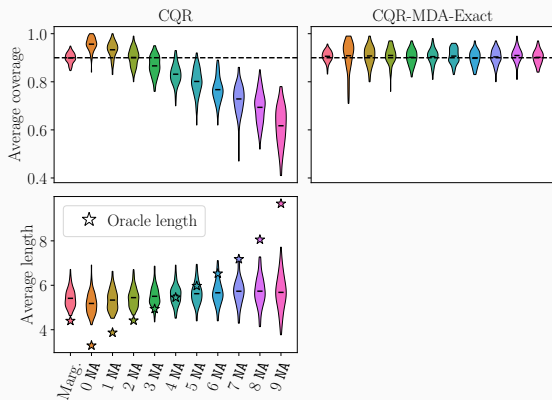
Synthetic experiments (Gaussian linear model, $d = 10$)



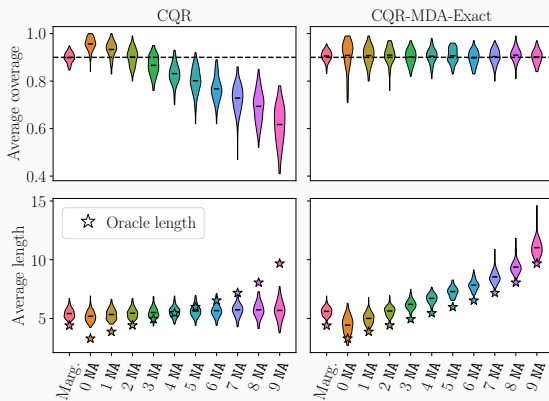
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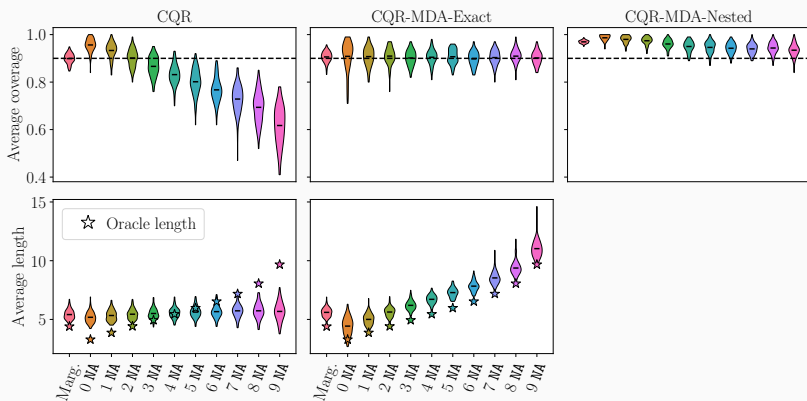
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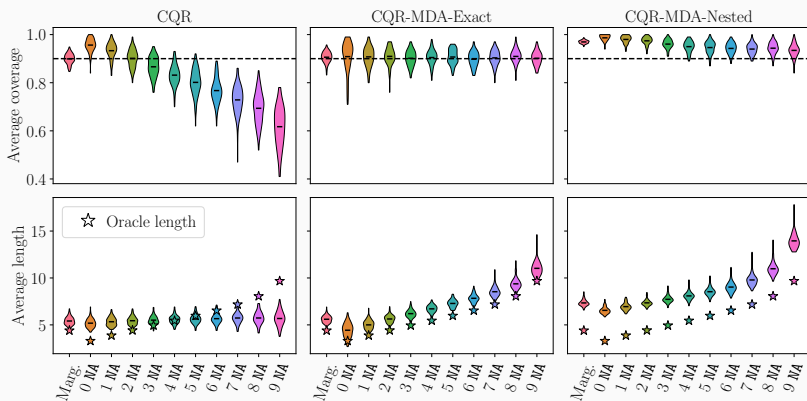
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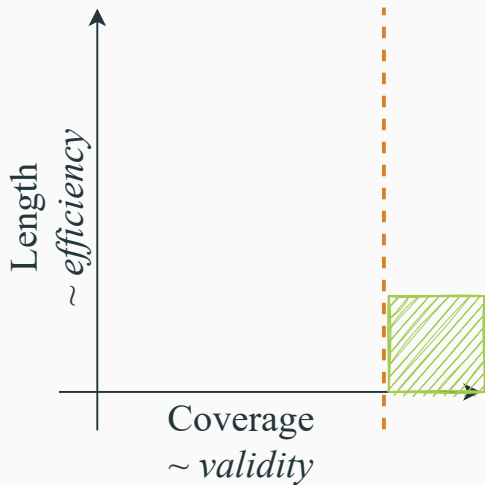
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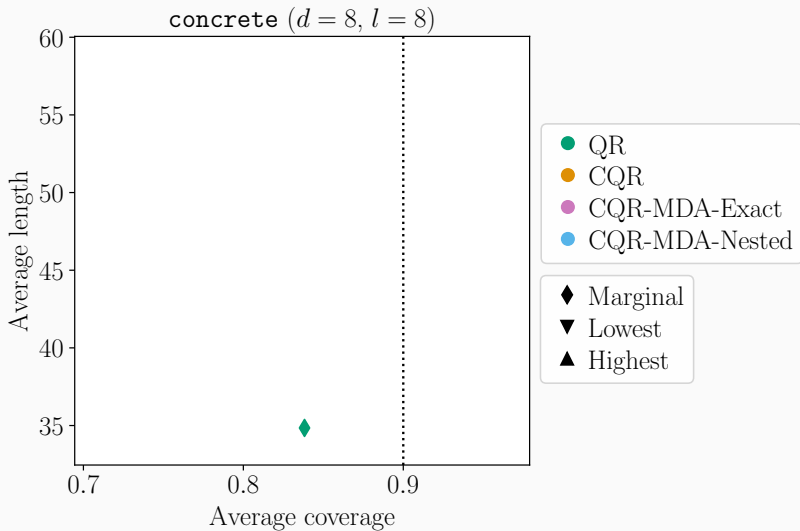
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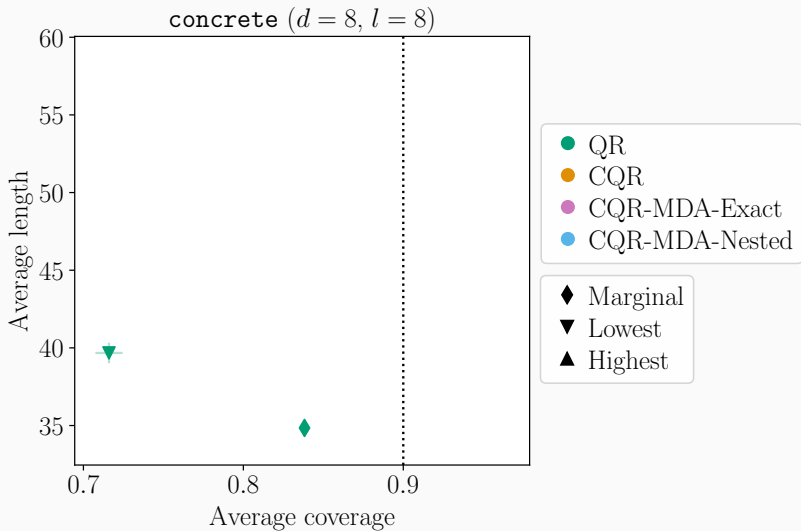
Before more experiments, visualisation



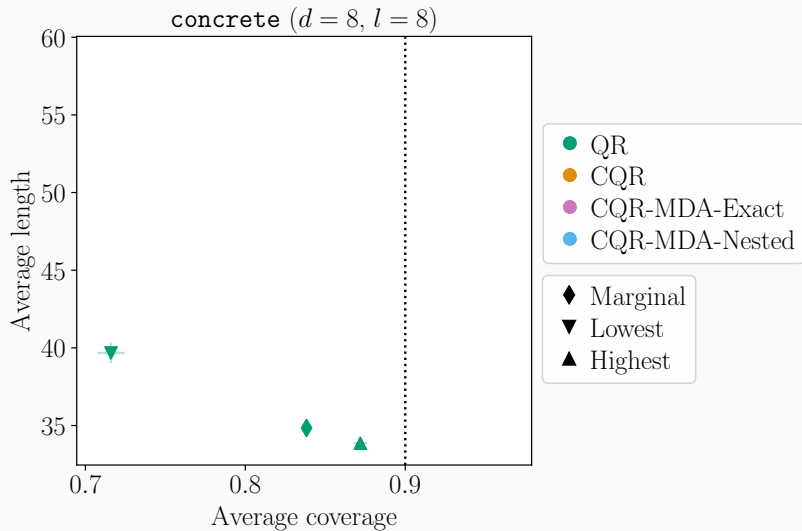
Semi-synthetic experiments



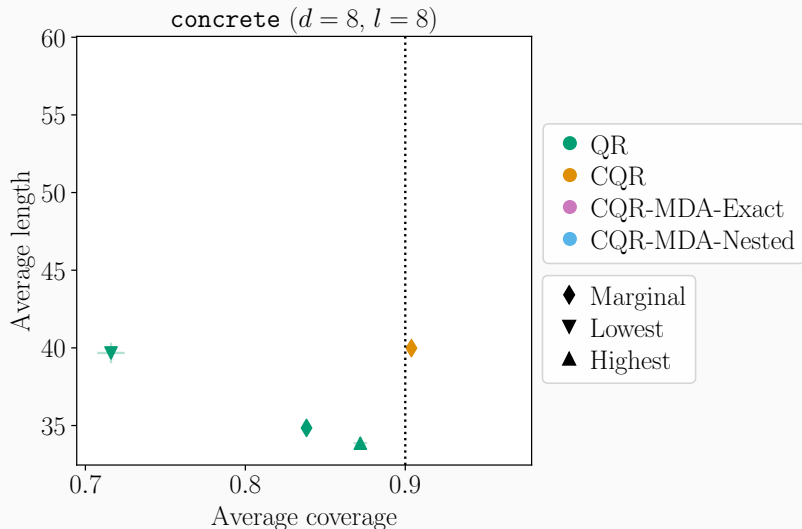
Semi-synthetic experiments



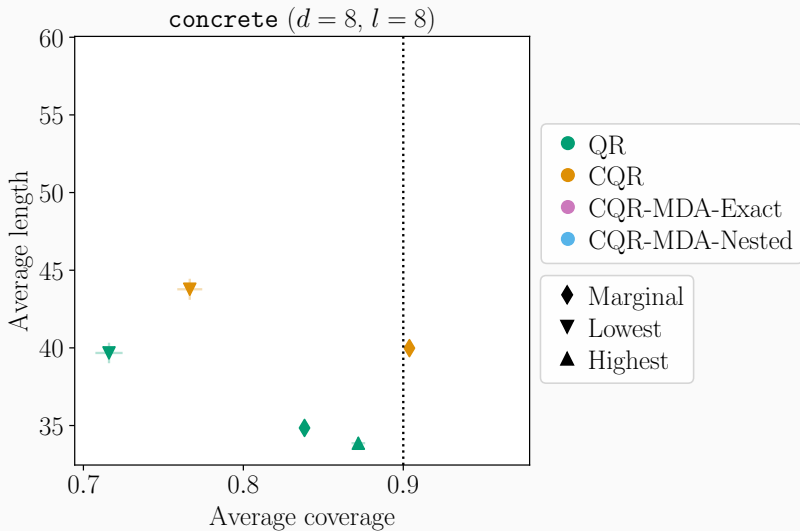
Semi-synthetic experiments



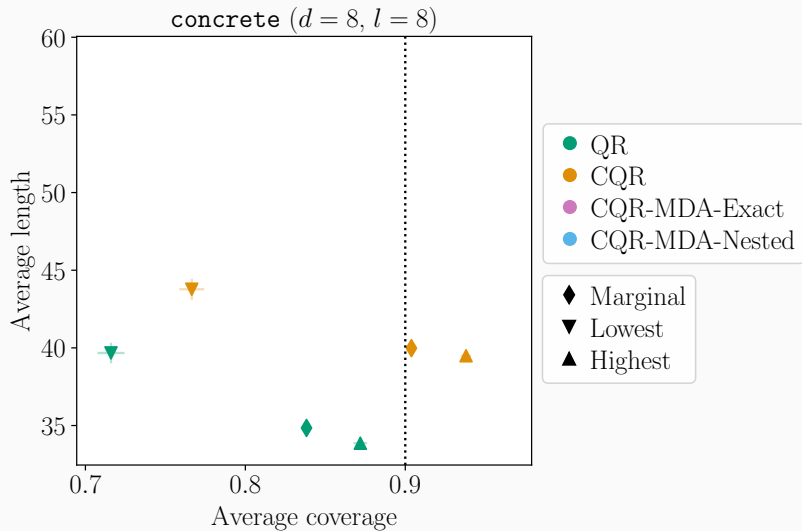
Semi-synthetic experiments



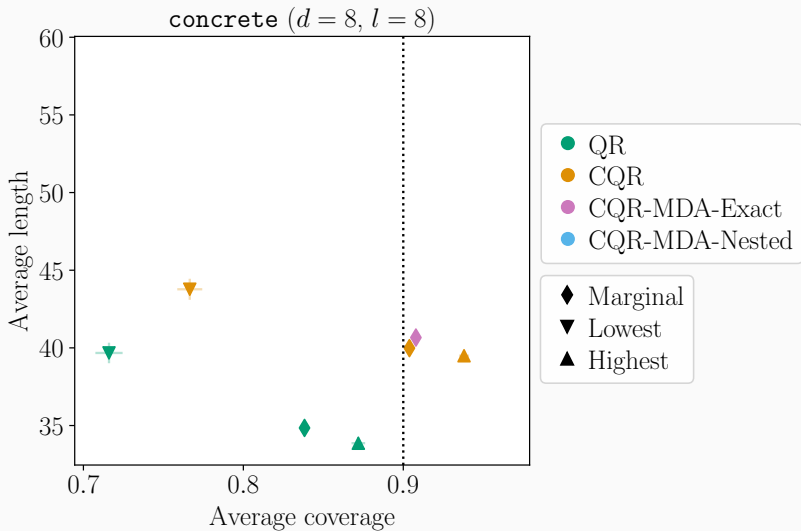
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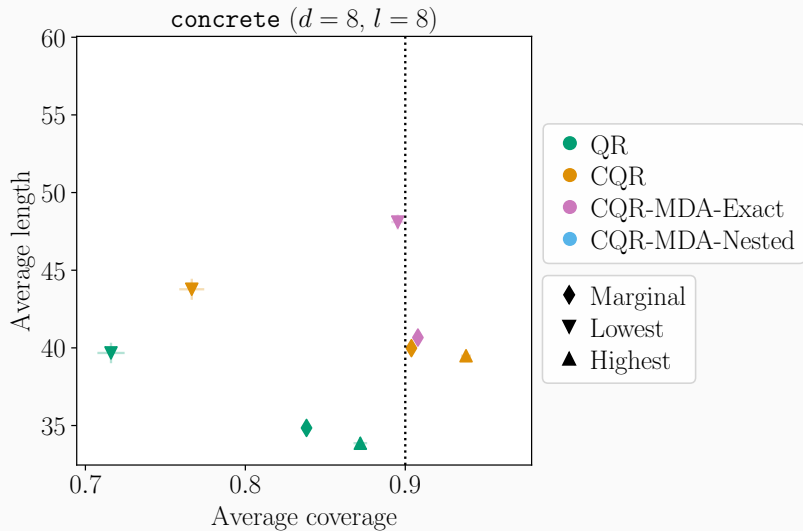
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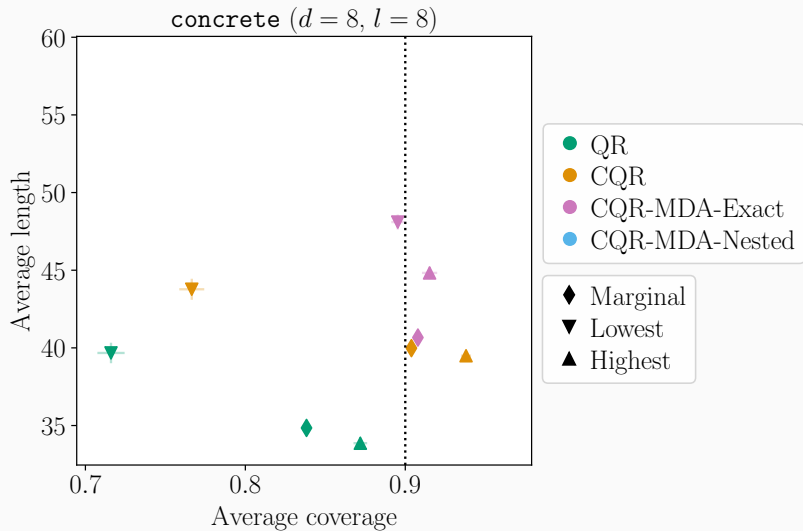
Semi-synthetic experiments



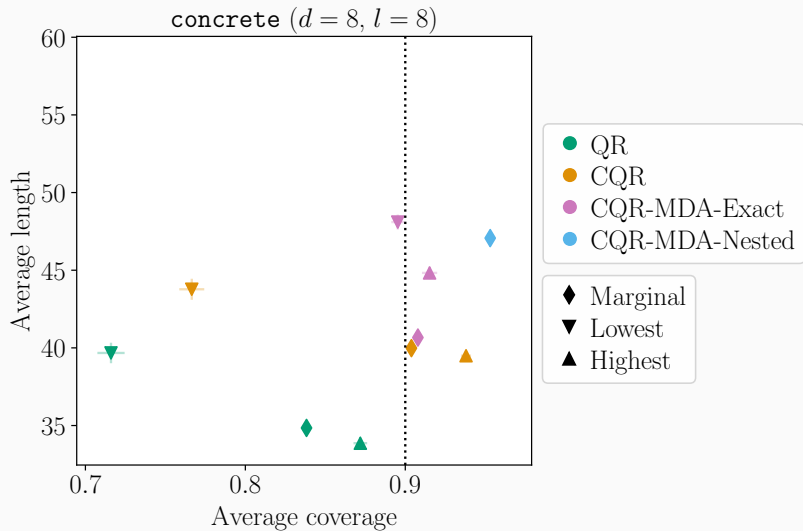
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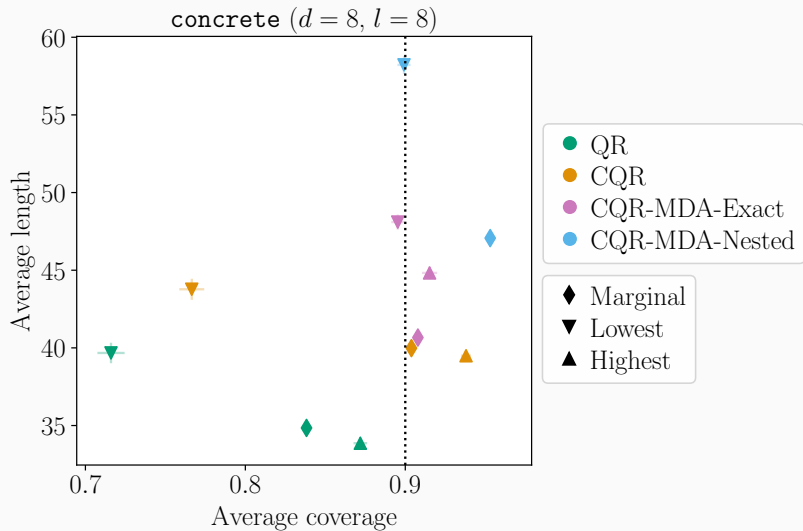
Semi-synthetic experiments



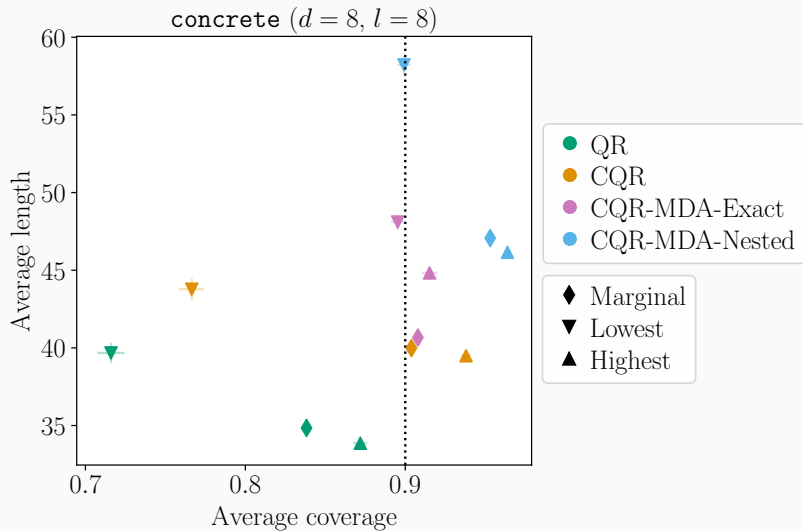
Semi-synthetic experiments



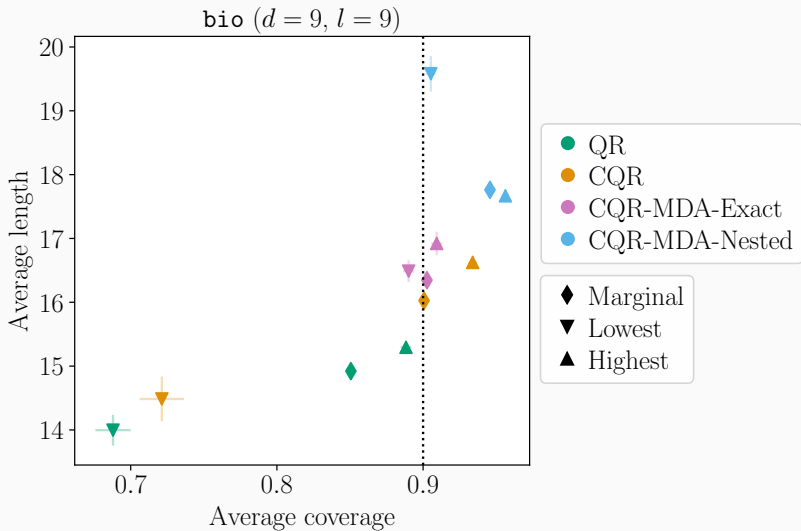
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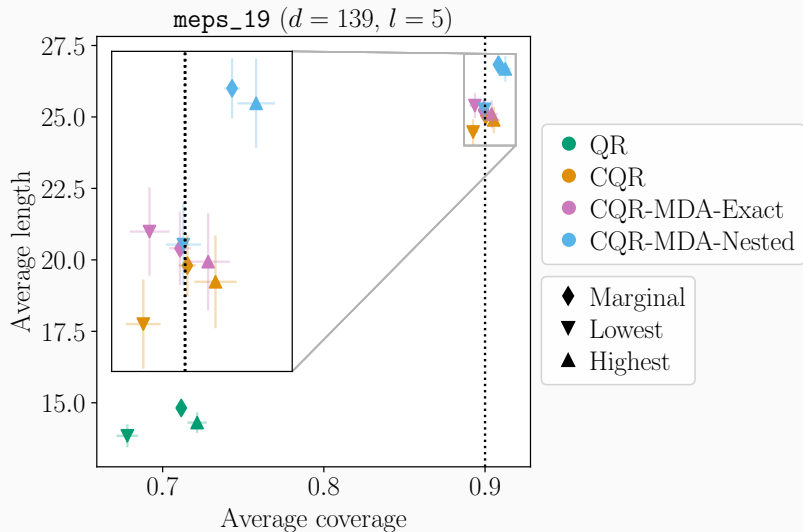
Semi-synthetic experiments



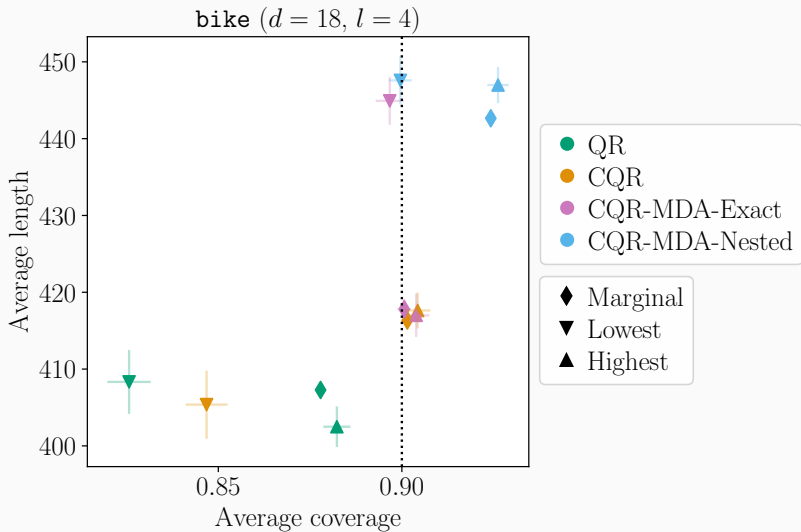
Semi-synthetic experiments



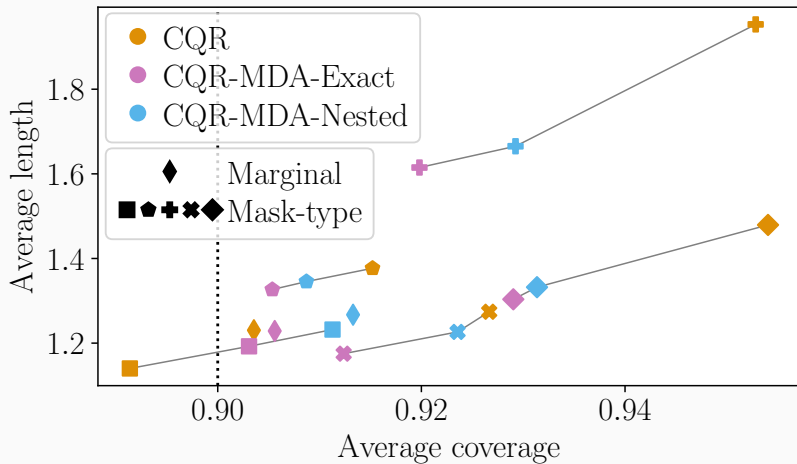
Semi-synthetic experiments



Semi-synthetic experiments



Real data experiment: back to critical care medicine



Conclusion

- CP marginal guarantees hold on the imputed data set.

Take-home-messages

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- CP marginal guarantees hold on the imputed data set.
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- **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

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
$\tilde{x}^{(3)}$	[Hatched area]			
$\tilde{x}^{(4)}$	0	NA	NA	1

What if we kept all individuals?

Test point

3	NA	NA	1
---	----	----	---

Initial calibration set

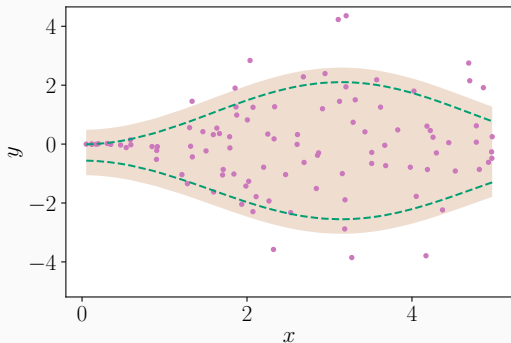
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$\tilde{x}^{(2)}$	4	NA	NA	2
$\tilde{x}^{(3)}$	5	NA	NA	NA
$\tilde{x}^{(4)}$	0	NA	NA	1

What if we kept all individuals?



► Predict with \hat{q}_{inf} and \hat{q}_{sup}

► Build $\hat{C}_{\hat{\alpha}}(x)$:

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

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

Temporary test points

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

and

CQR-MDA with nested masking in words

1. For a test point $(x^{(n+1)}, m^{(n+1)})$:
 - 1.1 For each $j \in \llbracket 1, d \rrbracket$ such that $m_j^{(n+1)} = 1$, set $\tilde{m}_j^{(k)} = 1$ (i.e. set $\tilde{x}_j^{(k)} = \text{NA}$) for k in the calibration set **such that**
 $m^{(k)} \subset m^{(n+1)}$

CQR-MDA with nested masking in words

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CQR-MDA with nested masking in words

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

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1. For a test point $(x^{(n+1)}, m^{(n+1)})$:
 - 1.1 Set $\tilde{m}^{(k)} = \max(m^{(k)}, m^{(n+1)})$ for k in the calibration set
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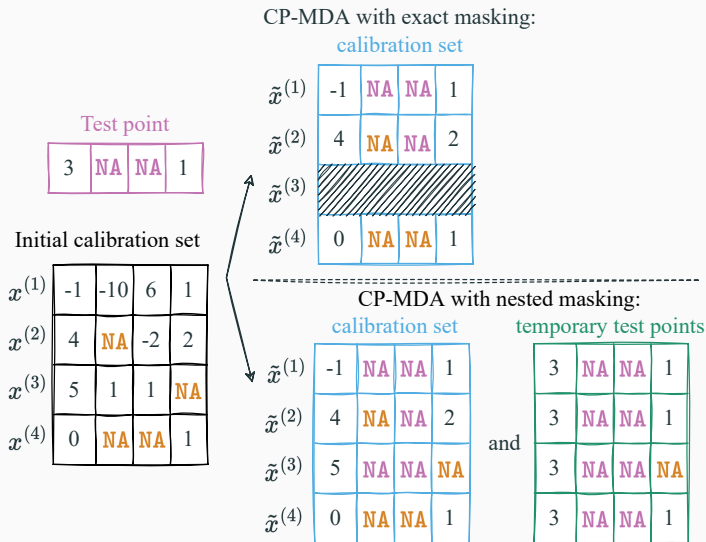
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Summary of CP-MDA



Towards asymptotic individualized coverage

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

Denote

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

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

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

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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 C^∞ imputation function Φ , if $F_{Y|(X_{\text{obs}(M)}, M)}$ 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

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$\Leftrightarrow \mathbb{P}(Y \in \hat{C}_\alpha(x) | X = x, M = m) \geq 1 - \alpha$ 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

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

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

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

Data generation

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

$$Y = \beta X + \varepsilon$$

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

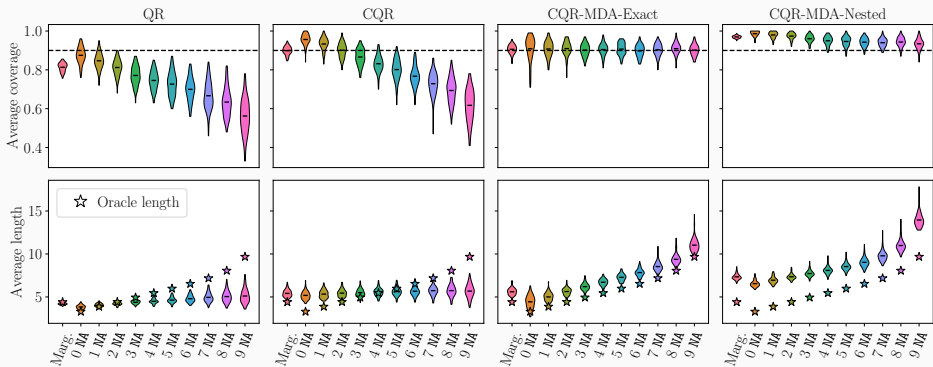
$$\text{and } (X_1, \dots, X_{10}) \sim \mathcal{N} \left(\begin{pmatrix} 1 \\ \vdots \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} 1 & 0.8 & \dots & 0.8 \\ 0.8 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0.8 \\ 0.8 & \dots & 0.8 & 1 \end{pmatrix} \right).$$

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

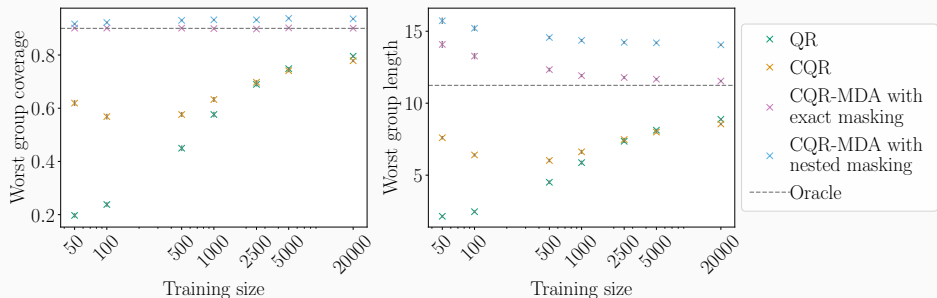
Results per pattern size



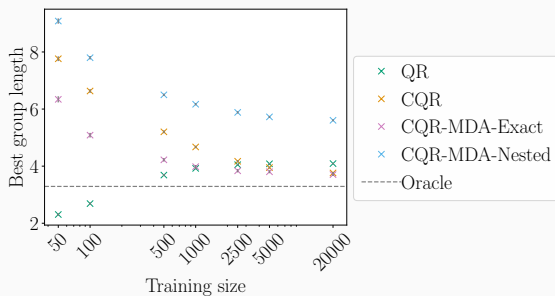
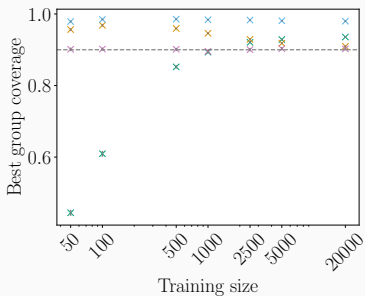
Simulation settings: varying training size

- Method: CQR
- Basemodel: neural network
- Imputation: iterative (\approx 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

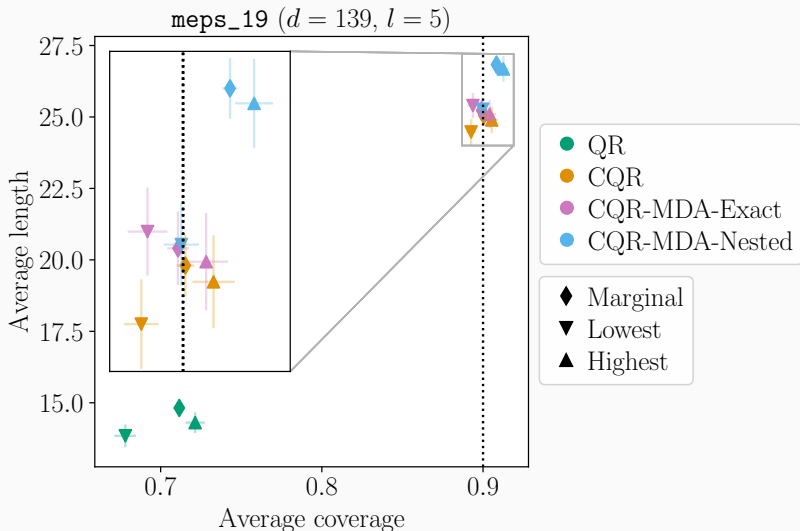


Results on the best group

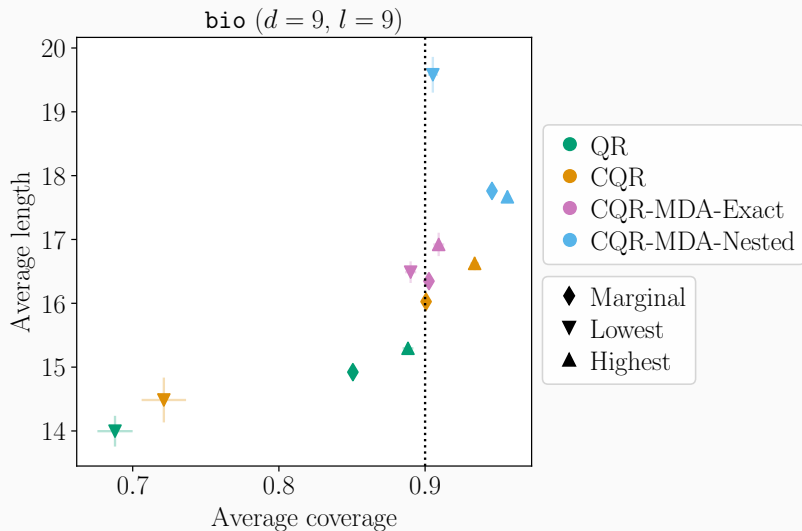


**Semi-synthetic experiments with
CQR-MDA-Nested**

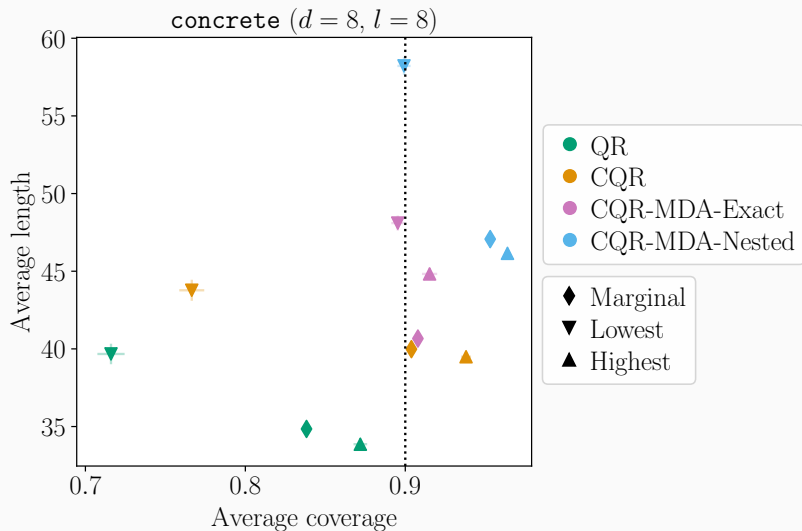
Semi-synthetic experiments with the CQR-MDA-Nested



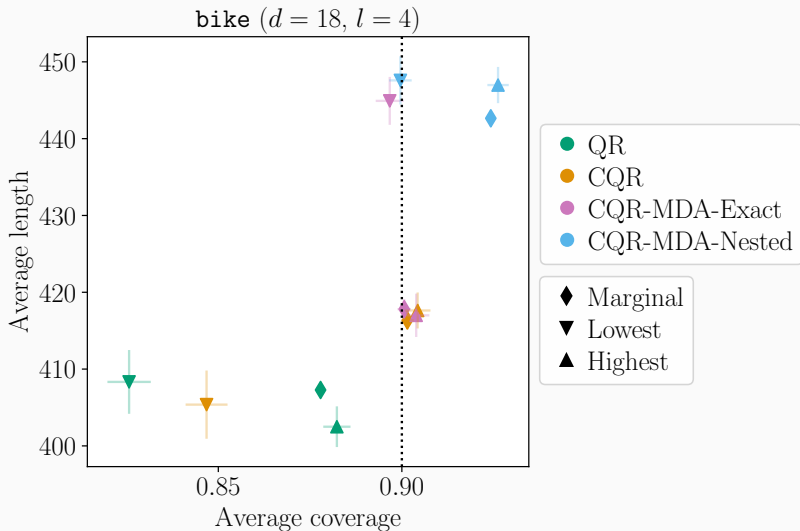
Semi-synthetic experiments with the CQR-MDA-Nested



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 $SI = \frac{HR}{SBP}$, 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

