Conformal Prediction with Missing Values

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joint work with Margaux Zaffran, Julie Josse, Yaniv Romano

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TraumaBase®: decision support for trauma patients

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- 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

Data: $\left(X^{(k)}, Y^{(k)}\right)_{k=1}^{n} \in \left(\mathbb{R}^{d} \times \mathbb{R}\right)^{n}$

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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
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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.*[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.

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Example

We observe $(\texttt{NA}, 6, 2)$. Then $m = (1, 0, 0)$ and $X_{\text{obs}(m)} = (6, 2)$.

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

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  $\hookrightarrow$ **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.

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Supervised learning with missing values: impute-then-regress

Impute-then-regress procedures are widely used.

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

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

$\xrightarrow{\phi}$

$u^{(1)}$	-1	-10	6	0
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$u^{(3)}$	5	1	2	1
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✓ Le Morvan et al. (2021)[3] show that for **any deterministic imputation** and **universal learner** this procedure is **Bayes-consistent**.

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✗ Ayme et al. (2022)[4] show that even for very **simple distributions** (linear model, Gaussian noise), this rate of convergence may suffer from **curse of dimensionality**.

[3] Le Morvan, Josse, Scornet & Varoquaux (2021), *What's a good imputation to predict with missing values?*, NeurIPS

[4] Ayme, Boyer, Dieuleveut & Scornet (2022), *Near-optimal rate of consistency for linear models with missing values*, ICML

Predictive uncertainty quantification with missing values

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

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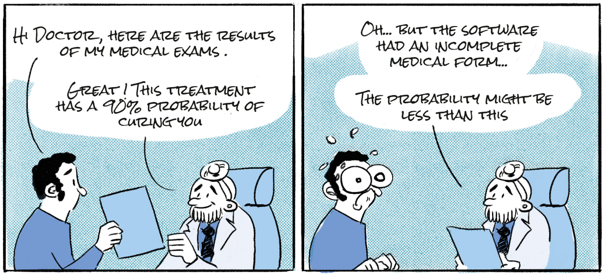
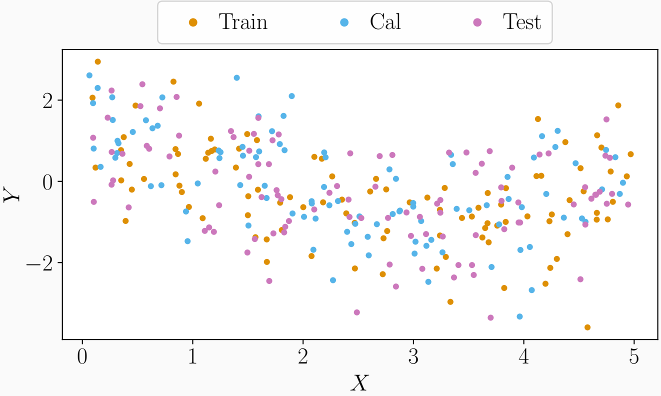
2. Mask-Conditional-Validity (MCV)

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



Illustrations @theo.remlinger

Split Conformal Prediction (Vovk et al., 2005): scheme



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

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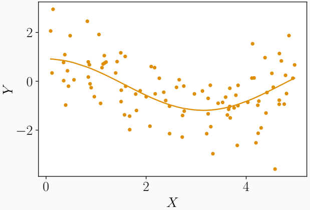
1) 

- Learn $\hat{\mu}$.

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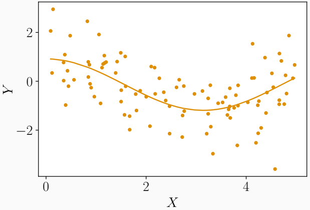

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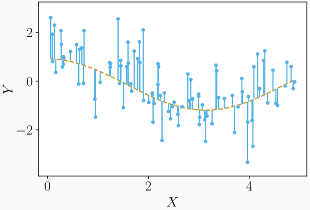

- Predict with $\hat{\mu}$.
- Get the residuals $\hat{\varepsilon}_i$ and form the set of scores $\mathcal{S} = \{|\hat{\varepsilon}_i|, i \in \mathrm{Cal}\} \cup \{+\infty\}$.
- Get their $(1 - \alpha)$ empirical quantile: $Q_{1-\alpha}(\mathcal{S})$.

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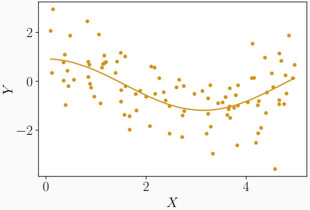

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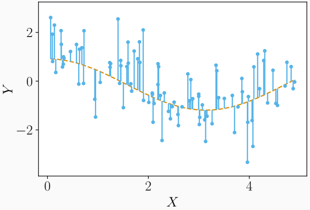

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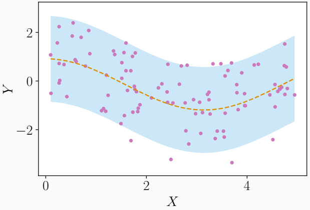
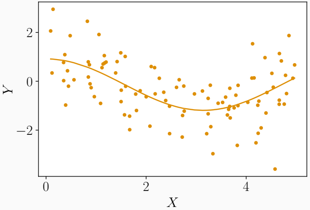
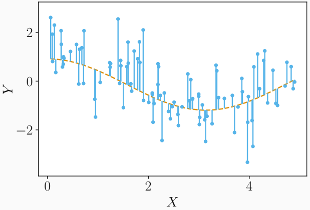


- Predict with $\hat{\mu}$.
- Build $\hat{C}_\alpha(x)$: $[\hat{\mu}(x) \pm Q_{1-\alpha}(\mathcal{S})]$.

1)


2
0
−2
Y
0
2
4
X

2)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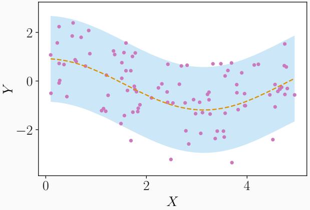
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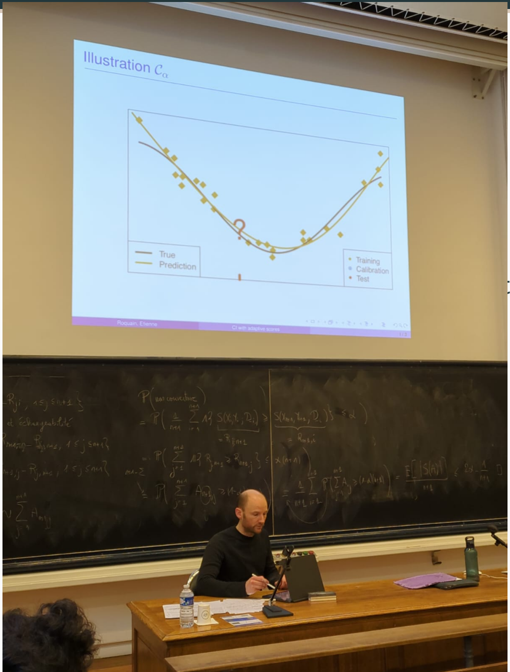
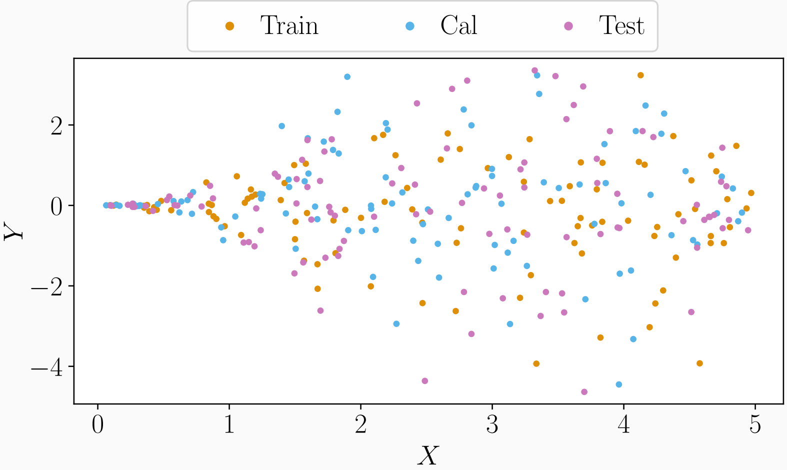


Illustration $\mathcal{C}_\alpha$
True
Prediction
Training
Calibration
Test

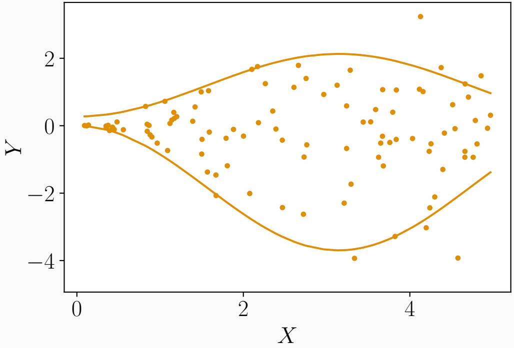
of

Conformalized Quantile Regression (CQR)[4]: toy example



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

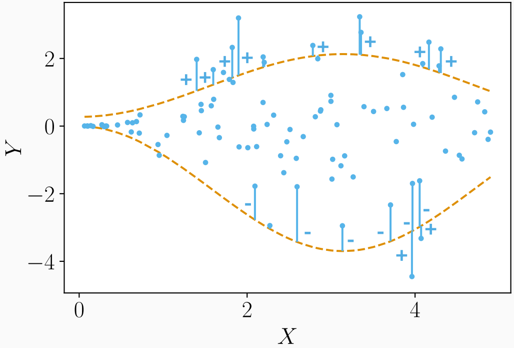
Conformalized Quantile Regression (CQR)[4]: training step



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

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

Conformalized Quantile Regression (CQR)[4]: calibration step



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

$$\hookrightarrow \quad S^{(k)} := \max\left\{\widehat{QR}_{\text{lower}}\left(X^{(k)}\right) - Y^{(k)}, Y^{(k)} - \widehat{QR}_{\text{upper}}\left(X^{(k)}\right)\right\}$$

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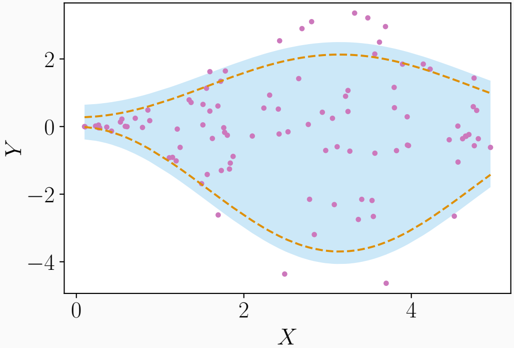
Conformalized Quantile Regression (CQR)[4]: prediction step



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

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

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

CQR: theoretical guarantees

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

Theorem

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

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

Additionally, if the scores $\left\{S^{(k)}\right\}_{k \in \mathrm{Cal}}$ *are a.s. distinct:*

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

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✓Finite sample

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

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3. On the calibration set, obtain $\#\mathrm{Cal} + 1$ conformity scores

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

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

Bonus - SCP: theoretical guarantees

This procedure enjoys the finite sample guarantee proposed and proved in Vovk et al. (2005).

Theorem

Suppose $(X_i, Y_i)_{i=1}^{n+1}$ *are exchangeable*[5]. *SCP on* $(X_i, Y_i)_{i=1}^{n}$ *outputs* $\widehat{C}_\alpha(\cdot)$ *such that:*

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If, in addition, the scores $\{S_i\}_{i \in \mathrm{Cal}} \cup \{S_{n+1}\}$ *are almost surely distinct, then*

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Proof: application of the quantile lemma.

[5] Only the calibration and test data need to be exchangeable.

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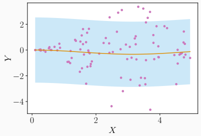
Visu.			
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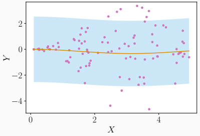
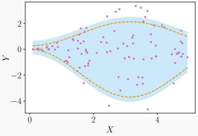
Visu.			
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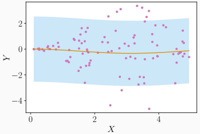
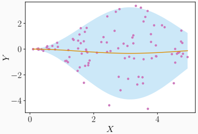
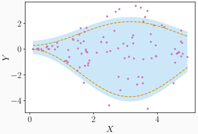
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)]$	$[\widehat{\text{QR}}_{\text{lower}}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{\text{QR}}_{\text{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
Visu.			
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CP is marginally valid (MV) after imputation

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

Lemma (Z. et al. (2023a))

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[6] ϕ*:*

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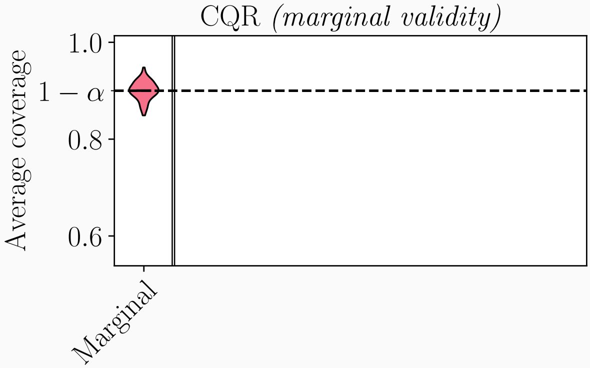

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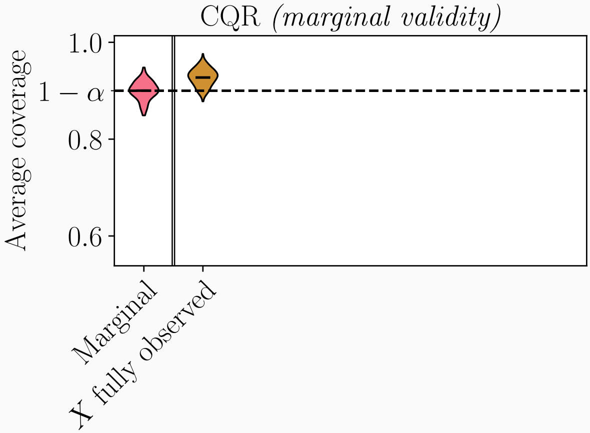

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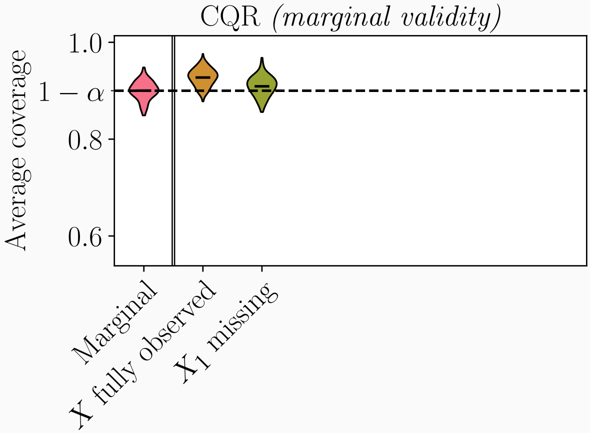

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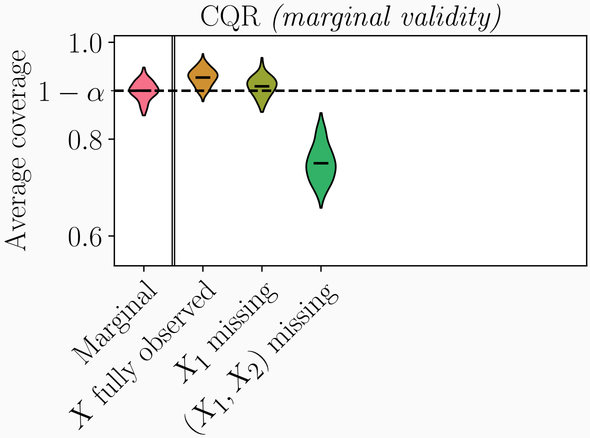

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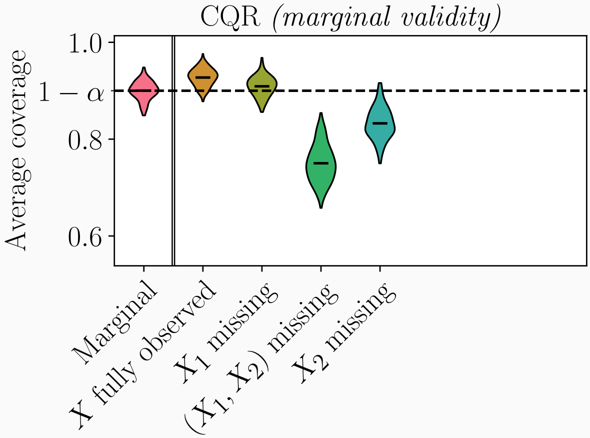

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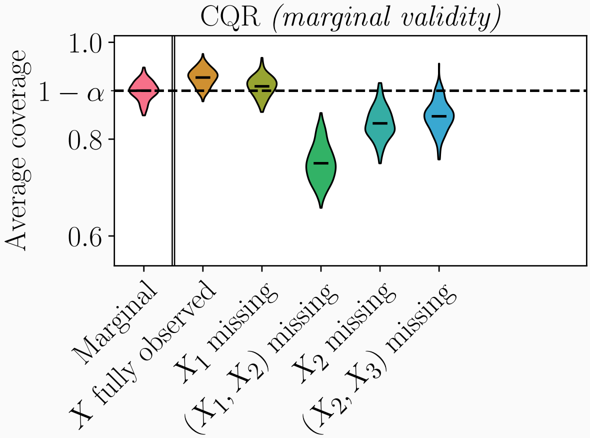

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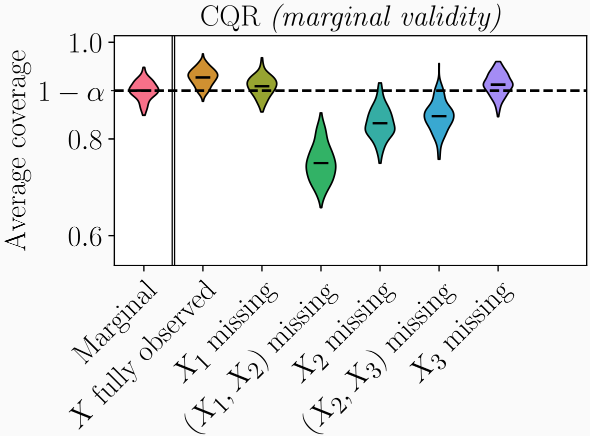

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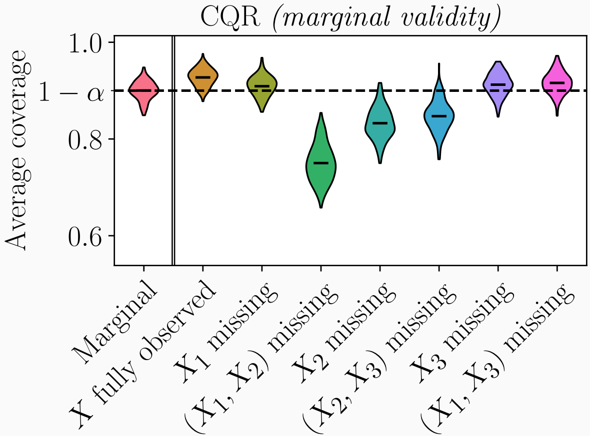

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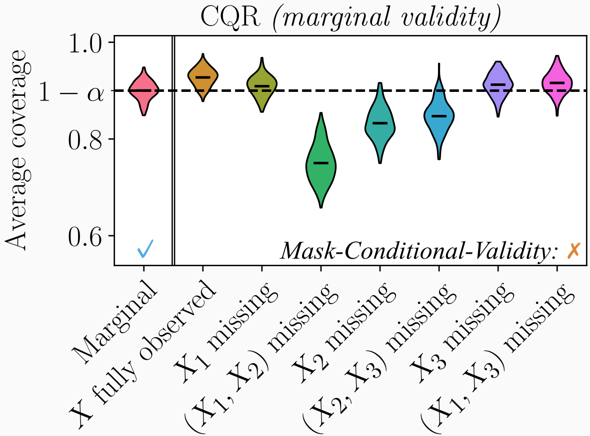

Warning: the predictive intervals cover properly **marginally**, but suffer from high **disparities depending on the missing patterns**.

Missing values induce heteroskedasticity

Gaussian linear model

- $Y = \beta^T X + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2) \perp\!\!\!\perp (X, M)$, $\beta \in \mathbb{R}^d$.
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$$\mathcal{L}_\alpha^*(m) = 2 \times q_{1-\alpha/2}^{\mathcal{N}(0,1)} \times \sqrt{\beta_{\mathrm{mis}(m)}^T \Sigma_{\mathrm{mis|obs}}^m \beta_{\mathrm{mis}(m)} + \sigma_\varepsilon^2}.$$

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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)**

Goals reminder: achieve MCV!

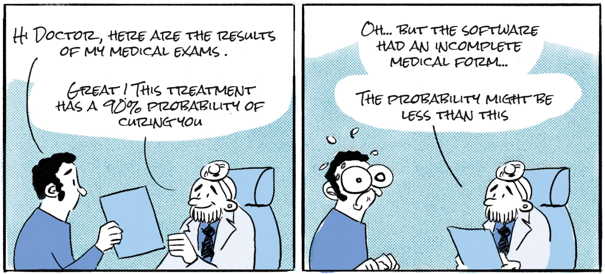
Goal: predict $Y^{(n+1)}$ with **confidence** $1-\alpha$, i.e. build the smallest $\mathcal{C}_\alpha$ such that:

1. Marginal Validity (MV) ✓

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

2. Mask-Conditional-Validity (MCV) ✗

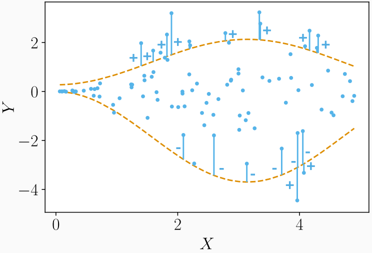
$$\forall m \in \{0,1\}^d : \mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, m\right) | M^{(n+1)} = m\right\} \geq 1-\alpha. \quad \text{(MCV)}$$



Illustrations @theo.remlinger

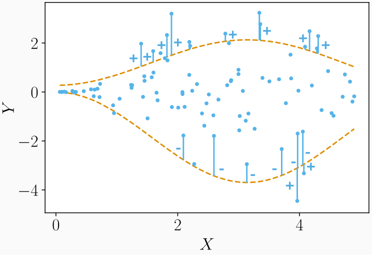
Conformalization step is independent of the important variable: the mask!

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



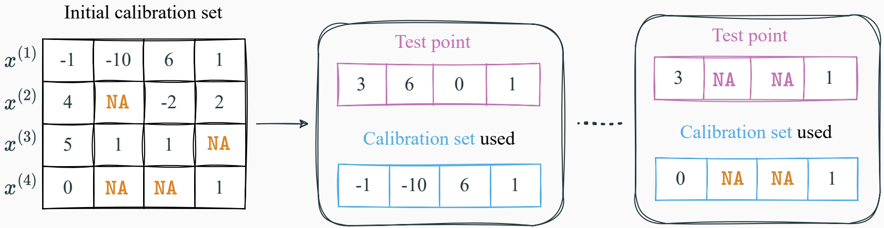
Conformalization step is independent of the important variable: the mask!

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

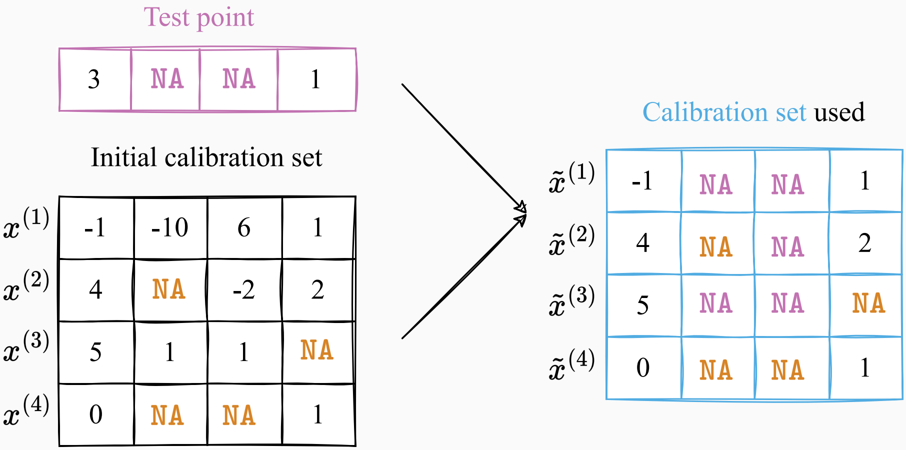


Warning: 2^d possible masks

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



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



Algorithms: MDA with Exact masking or with Nested masking.

CP-MDA with Exact masking

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

CP-MDA with Exact masking

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

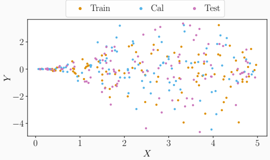
Calibration set used

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

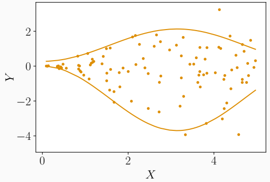
$\#\mathrm{Cal}^{\mathrm{M}^{(\text{test})}}$ observations

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`

CQR-MDA with exact masking in words

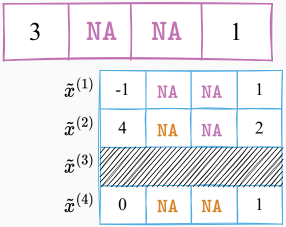
1. Split the training set into a `proper training set` and `calibration set`
2. Train the imputation function on the `proper training set`
3. Impute the `proper training set`
4. Train the quantile regressors on the `imputed proper training set`
5. For a test point $(X^{(n+1)}, M^{(n+1)})$:

3	NA	NA	1

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 $(X^{(n+1)}, M^{(n+1)})$:

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



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`
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   5.2 Impute the new `calibration set`

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

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`
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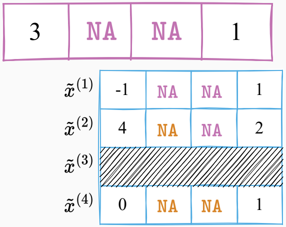
   5.2 Impute the new `calibration set`

   5.3 Compute the calibration correction, i.e. $q_{1-\alpha}(\mathcal{S})$



CQR-MDA with exact masking in words

1. Split the training set into a `proper training set` and `calibration set`
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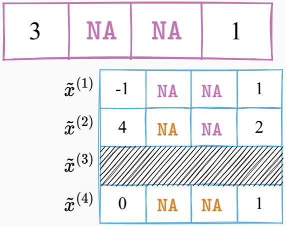
   5.2 Impute the new `calibration set`

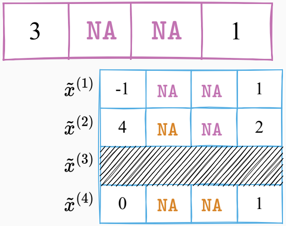
   5.3 Compute the calibration correction, i.e. $q_{1-\alpha}(\mathcal{S})$

   5.4 Impute the test point



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 $(X^{(n+1)}, M^{(n+1)})$:



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

   5.2 Impute the new `calibration set`

   5.3 Compute the calibration correction, i.e. $q_{1-\alpha}(\mathcal{S})$

   5.4 Impute the test point

   5.5 Predict with the quantile regressors and the correction previously obtained, $q_{1-\alpha}(\mathcal{S})$

MDA-Exact achieves Mask-Conditional-Validity (MCV)

Theorem (CP-MDA-Exact achieves MCV, Z. et al. (2023a))

If: i) the data is exchangeable, ii) $M \perp\!\!\!\perp X$, iii) $(Y \perp\!\!\!\perp M)|X$, then for almost all imputation function CP-MDA-Exact is such that for any $m \in \{0,1\}^d$:

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

and if additionally the scores are almost surely distinct:

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

What if we kept all observations?

Test point

3	NA	NA	1

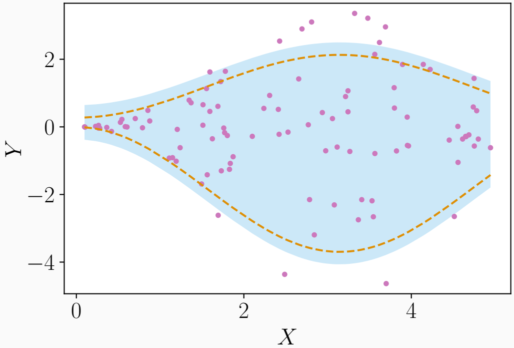
Initial calibration set

$x^{(1)}$	-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 observations?



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

- Build

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

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

$\rightsquigarrow$ similar motivation than Barber et al. (2021)[8] and Gupta et al. (2022)[9].

[8] *Predictive inference with the jackknife+*, The Annals of Statistics

[9] *Nested conformal prediction and quantile out-of-bag ensemble methods*, Pattern Recognition

CQR-MDA with nested masking in words

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

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

3	NA	NA	1

$\tilde{x}^{(1)}$	-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

CQR-MDA with nested masking in words

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

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

   5.2 Impute the new `calibration set`

   5.3 For each augmented calibration point k:

3	NA	NA	1

$\tilde{x}^{(1)}$	-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

CQR-MDA with nested masking in words

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

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

   5.2 Impute the new `calibration set`

   5.3 For each augmented calibration point k:

      5.3.1 Get its score $S^{(k)}$

3	NA	NA	1

$\tilde{x}^{(1)}$	-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

CQR-MDA with nested masking in words

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

3	NA	NA	1

5.1 Set $\tilde{M}^{(k)} = \max(M^{(k)}, M^{(n+1)})$ for k 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

5.2 Impute the new `calibration set`

5.3 For each augmented calibration point k:

5.3.1 Get its score $S^{(k)}$

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

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

CQR-MDA with nested masking in words

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

3	NA	NA	1

  5.1 Set $\tilde{M}^{(k)} = \max(M^{(k)}, M^{(n+1)})$ for k 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

  5.2 Impute the new `calibration set`

  5.3 For each augmented calibration point k:

    5.3.1 Get its score $S^{(k)}$

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

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

    5.3.3 Compute the corrected prediction interval:

$$[\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),k}) - S^{(k)}; \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k}) + S^{(k)}] := \left[Z^{(k)}_{\text{lower}}; Z^{(k)}_{\text{upper}}\right]$$

CQR-MDA with nested masking in words

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

3	NA	NA	1

$\tilde{x}^{(1)}$	-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

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

5.2 Impute the new `calibration set`

5.3 For each augmented calibration point k:

5.3.1 Get its score $S^{(k)}$

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

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

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$[\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),k}) - S^{(k)}; \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k}) + S^{(k)}] := \left[Z^{(k)}_{\text{lower}}; Z^{(k)}_{\text{upper}}\right]$

5.4 Compute the quantiles $q_\alpha(\{Z^{(k)}_{\text{lower}}\}_{k\in\mathrm{Cal}})$ and $q_{1-\alpha}(\{Z^{(k)}_{\text{upper}}\}_{k\in\mathrm{Cal}})$

CQR-MDA with nested masking in words

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

3	NA	NA	1

$\tilde{x}^{(1)}$	-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

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

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

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

5.3.3 Compute the corrected prediction interval:
$$[\widehat{QR}_{\alpha/2}(\tilde{X}^{(n+1),k}) - S^{(k)}; \widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k}) + S^{(k)}] := \left[Z^{(k)}_{\text{lower}}; Z^{(k)}_{\text{upper}}\right]$$

5.4 Compute the quantiles $q_\alpha(\{Z^{(k)}_{\text{lower}}\}_{k\in\mathrm{Cal}})$ and $q_{1-\alpha}(\{Z^{(k)}_{\text{upper}}\}_{k\in\mathrm{Cal}})$

5.5 Predict $[q_\alpha(\{Z^{(k)}_{\text{lower}}\}_{k\in\mathrm{Cal}}); q_{1-\alpha}(\{Z^{(k)}_{\text{upper}}\}_{k\in\mathrm{Cal}})]$

MDA-Nested is Marginally Valid (MV)

Theorem (CP-MDA-Nested marginal validity, Z. et al. (2023b))

If the data is exchangeable, then for almost all imputation function CP-MDA-Nested is such that:

$$\mathbb{P}\left(Y \in \widehat{C}_\alpha\left(X, M\right)\right) \geq 1 - 2\alpha.$$

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- ✓ Any missing mechanism (no need to assume $M \perp\!\!\!\perp X$)
- ✓ Does not require $(Y \perp\!\!\!\perp M)\,|X$
- ✗ Marginal guarantee

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- ✓ Any missing mechanism (no need to assume $M \perp\!\!\!\perp X$)
- ✓ Does not require $(Y \perp\!\!\!\perp M) | X$
- ✗ Marginal guarantee

Proof element: based on Jackknife+ ideas (Barber et al., 2021).

Leaving-out the k-th data point to predict on the l-th data point

$\leftrightarrow$

Apply the mask of the k-th data point to the l-th data point on which you predict

MDA-Nested (nearly) achieves Mask-Conditional-Validity (MCV)

Stochastic domination of the quantiles (SDQ)

Let $(\mathring{m}, \breve{m}) \in \left(\{0,1\}^d\right)^2$. If $\mathring{m} \subset \breve{m}$ then for any $\delta \in [0, 0.5]$: $q_{1-\delta/2}^{Y|(X_{\text{obs}(\mathring{m})}, M=\mathring{m})} \leq q_{1-\delta/2}^{Y|(X_{\text{obs}(\breve{m})}, M=\breve{m})}$, and $q_{\delta/2}^{Y|(X_{\text{obs}(\mathring{m})}, M=\mathring{m})} \geq q_{\delta/2}^{Y|(X_{\text{obs}(\breve{m})}, M=\breve{m})}$.

$\rightsquigarrow$ predictive uncertainty increases with bigger masks.

MDA-Nested (nearly) achieves Mask-Conditional-Validity (MCV)

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$\rightsquigarrow$ predictive uncertainty increases with bigger masks.

Theorem (CP-MDA-Nested (nearly) achieves MCV, Z. et al. (2023a))

If i) the data is exchangeable, ii) $M \perp\!\!\!\perp X$, iii) $(Y \perp\!\!\!\perp M)|X$, iv) SDQ holds, then for almost all imputation function "CP-MDA-Nested" is s.t. for any $m \in \{0,1\}^d$:

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

MDA-Nested (nearly) achieves Mask-Conditional-Validity (MCV)

Stochastic domination of the quantiles (SDQ)

Let $(\mathring{m}, \breve{m}) \in (\{0,1\}^d)^2$. If $\mathring{m} \subset \breve{m}$ then for any $\delta \in [0, 0.5]$: $q_{1-\delta/2}^{Y|(X_{\text{obs}(\mathring{m})}, M=\mathring{m})} \leq q_{1-\delta/2}^{Y|(X_{\text{obs}(\breve{m})}, M=\breve{m})}$, and $q_{\delta/2}^{Y|(X_{\text{obs}(\mathring{m})}, M=\mathring{m})} \geq q_{\delta/2}^{Y|(X_{\text{obs}(\breve{m})}, M=\breve{m})}$.

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Change on MDA-Nested: outputs any $[q_\alpha(\{Z_{\text{lower}}^{(k)}\}_{k \in \mathrm{Cal}^{\breve{m}}}); q_{1-\alpha}(\{Z_{\text{upper}}^{(k)}\}_{k \in \mathrm{Cal}^{\breve{m}}})]$, where $\breve{m}$ is randomly[10] selected such that $m \subset \breve{m}$.

[10] The randomness may depend on $\#\mathrm{Cal}^{\breve{m}}$.

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

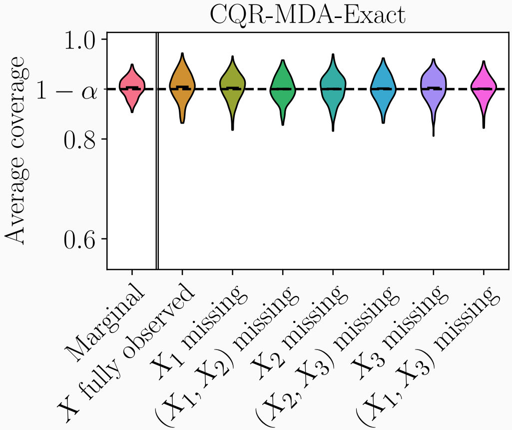
temporary test points

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

MDA achieves Mask-Conditional-Validity (MCV)

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

$\beta = (1, 2, -1)^T$, $\varepsilon \perp\!\!\!\perp X$, X and ε Gaussian, 20% uniform MCAR missing values.



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

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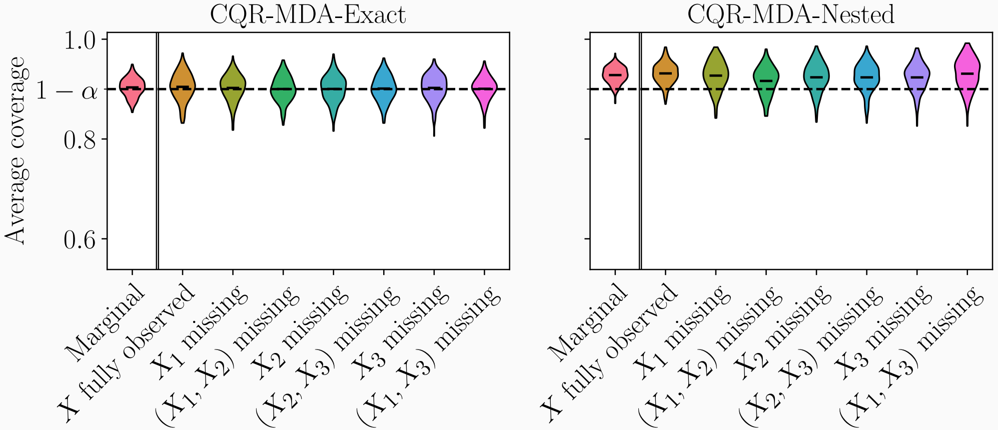

MDA achieves (MCV) in an informative way

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

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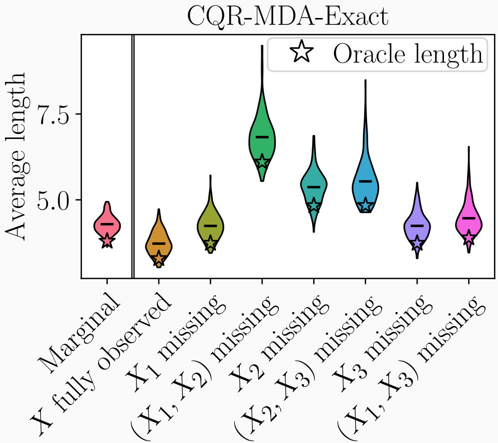

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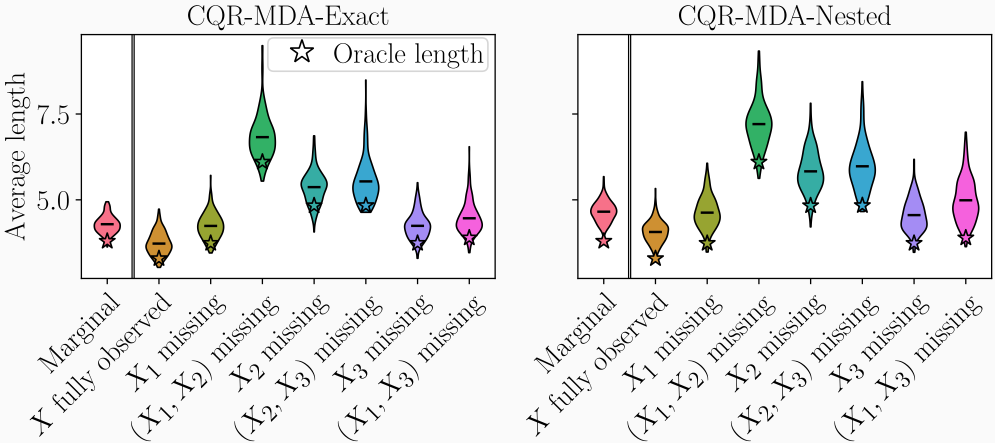

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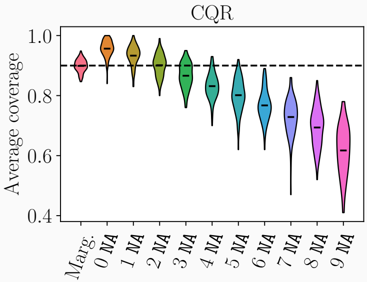
  - 100 repetitions

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



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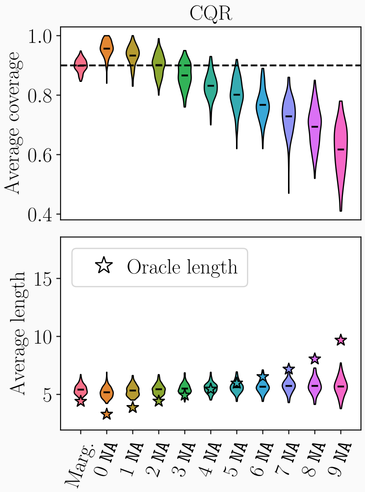

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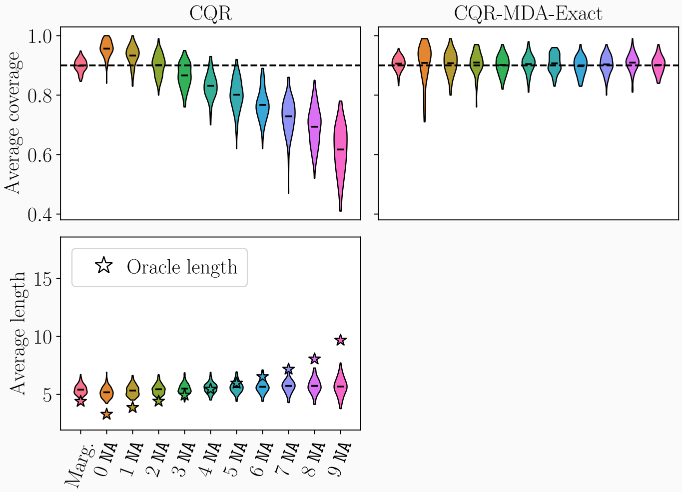

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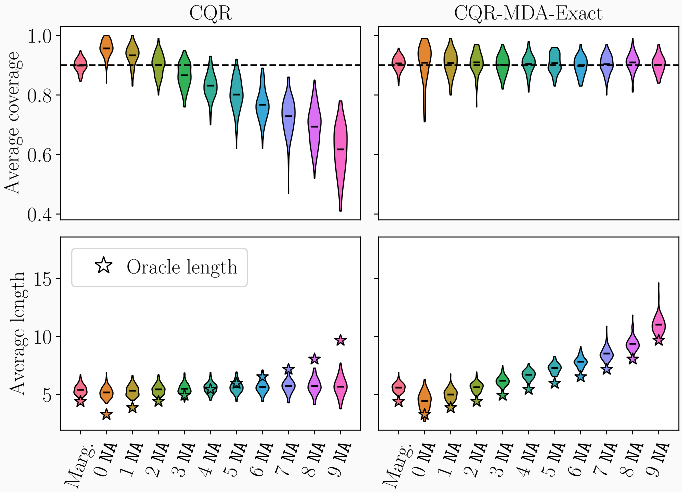

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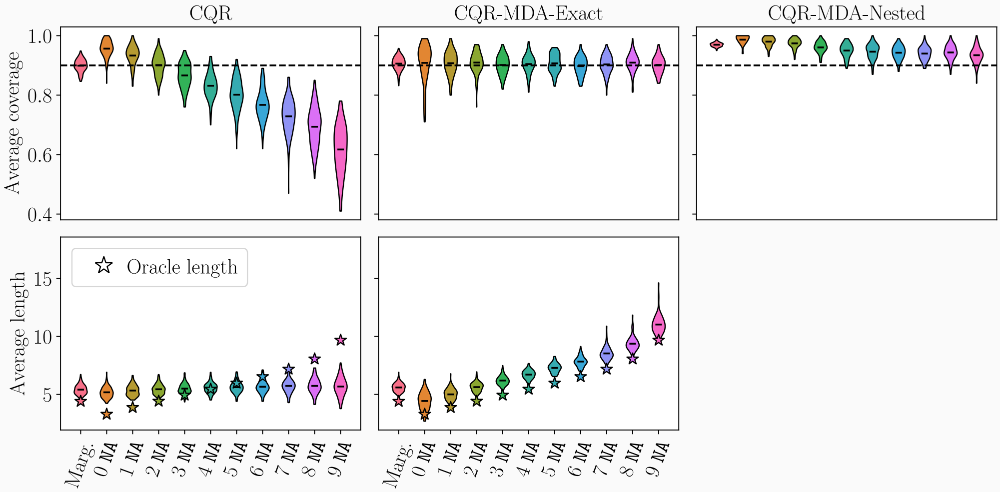

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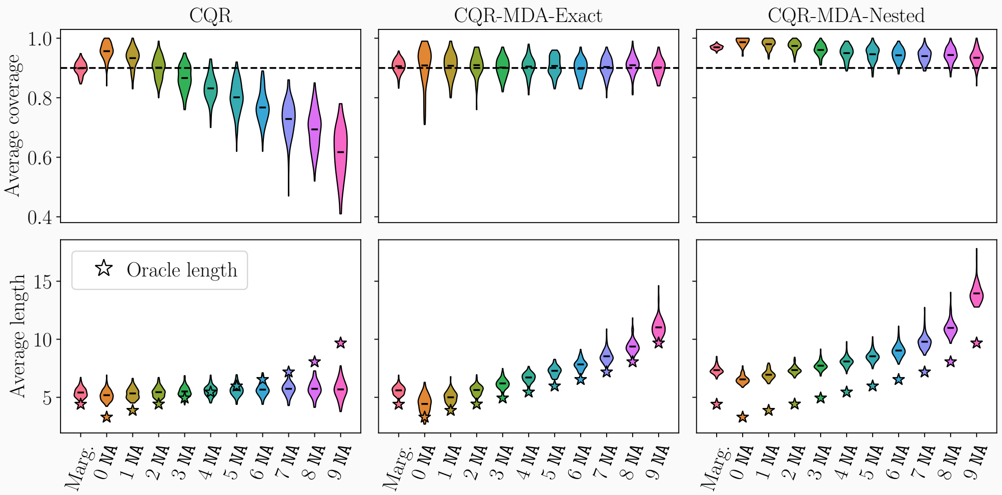
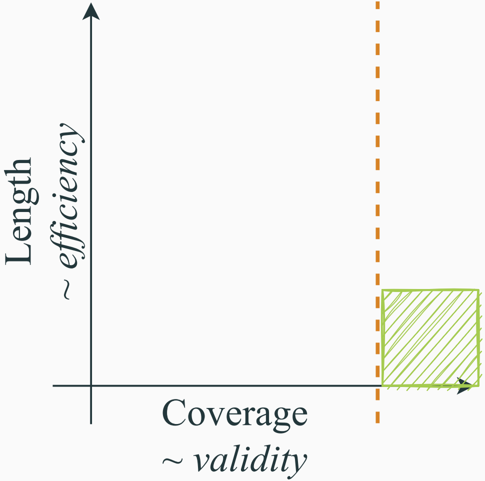
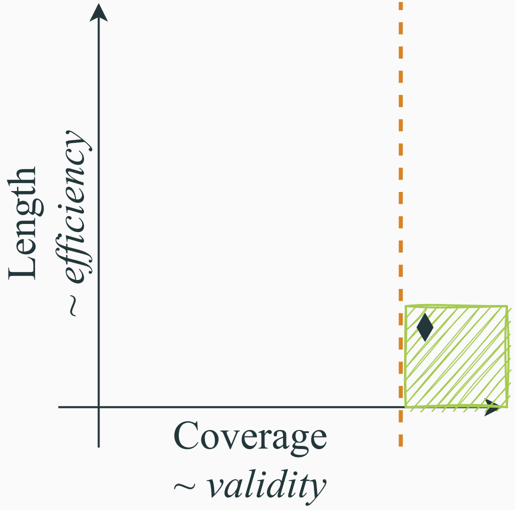


Before more experiments, visualisation





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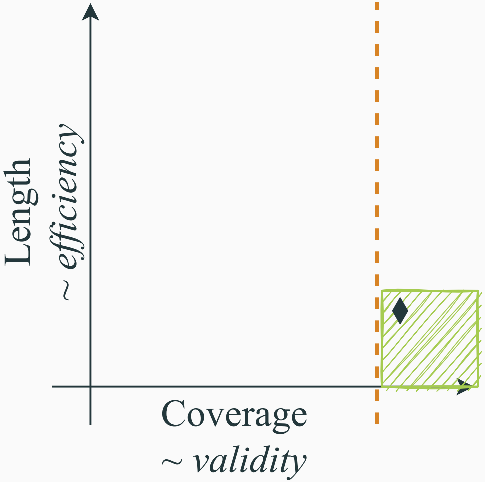

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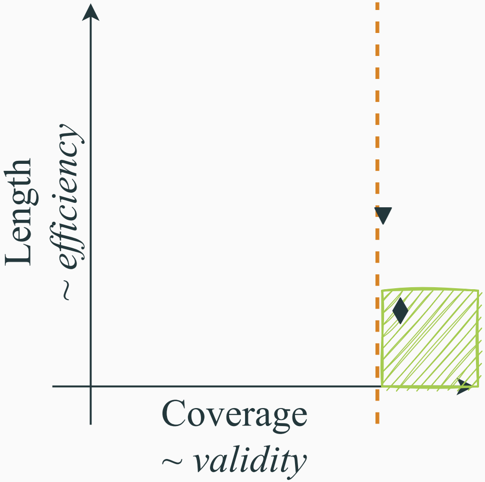

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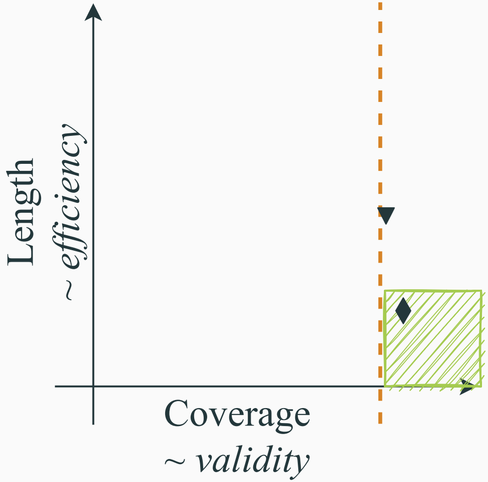

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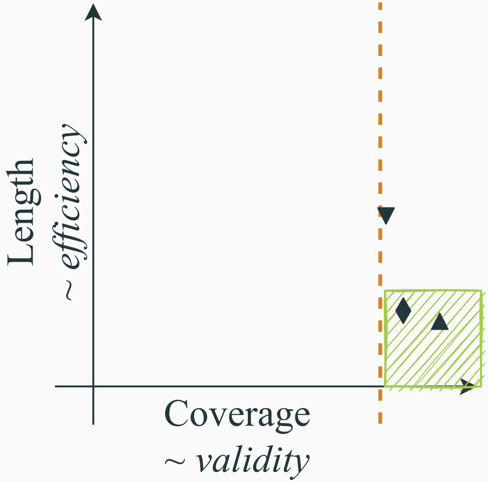

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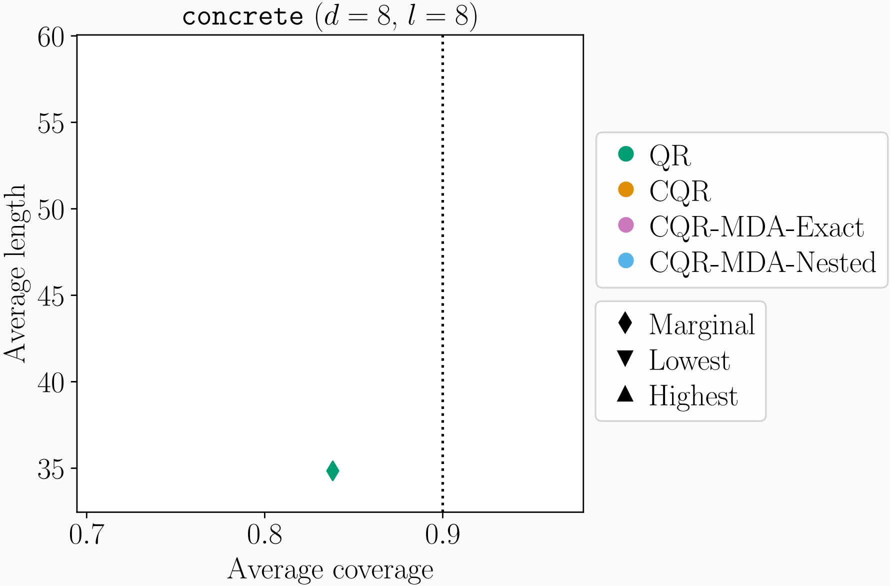

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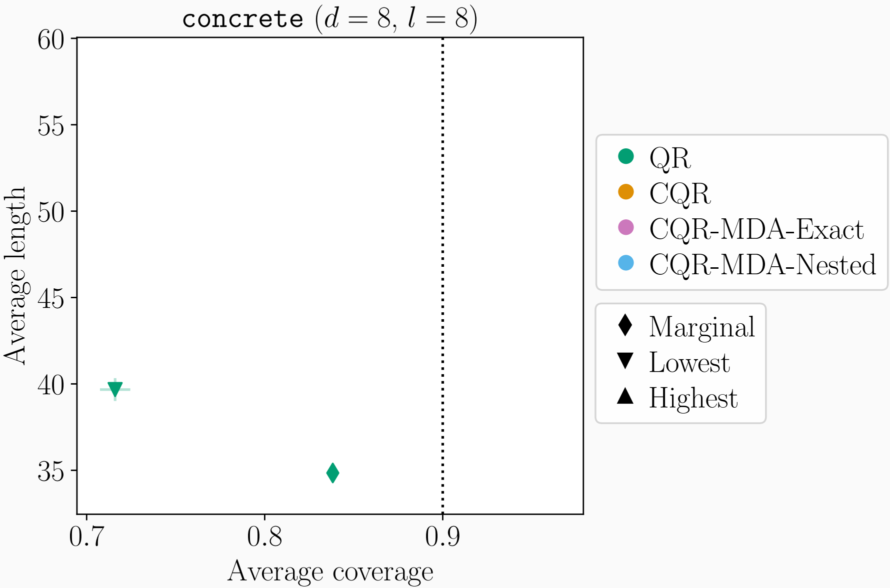

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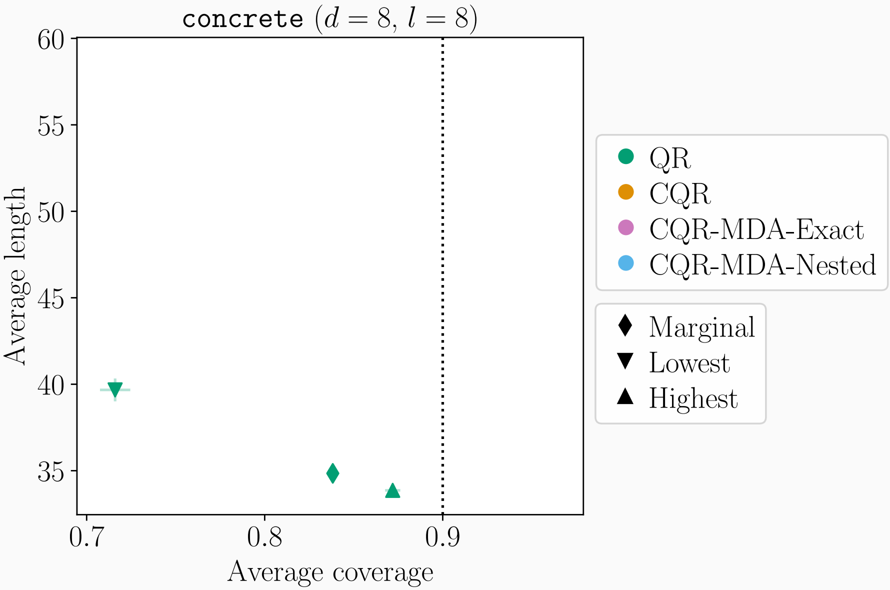

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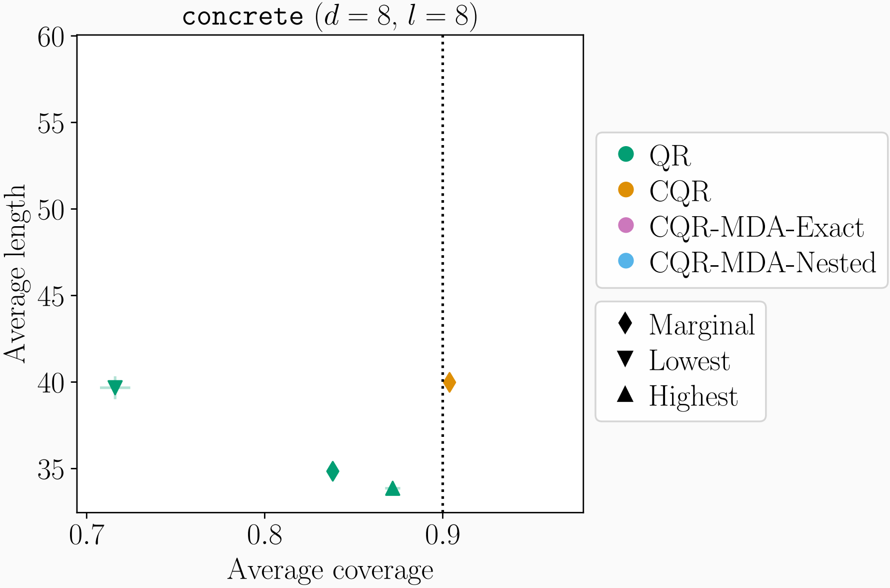

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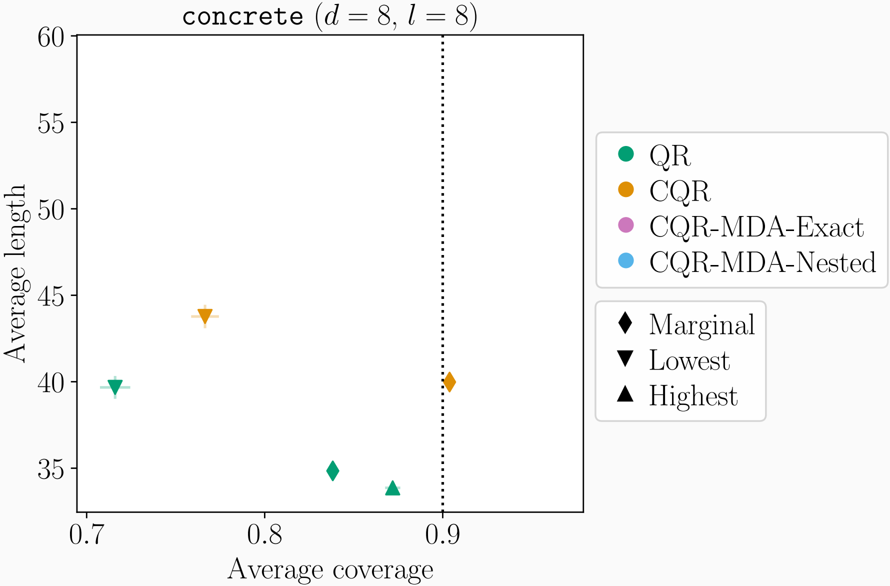

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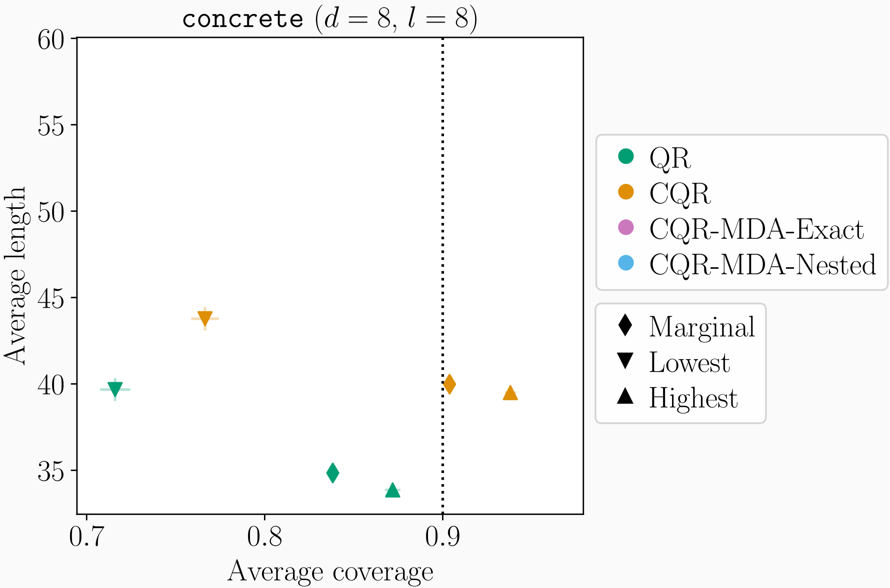

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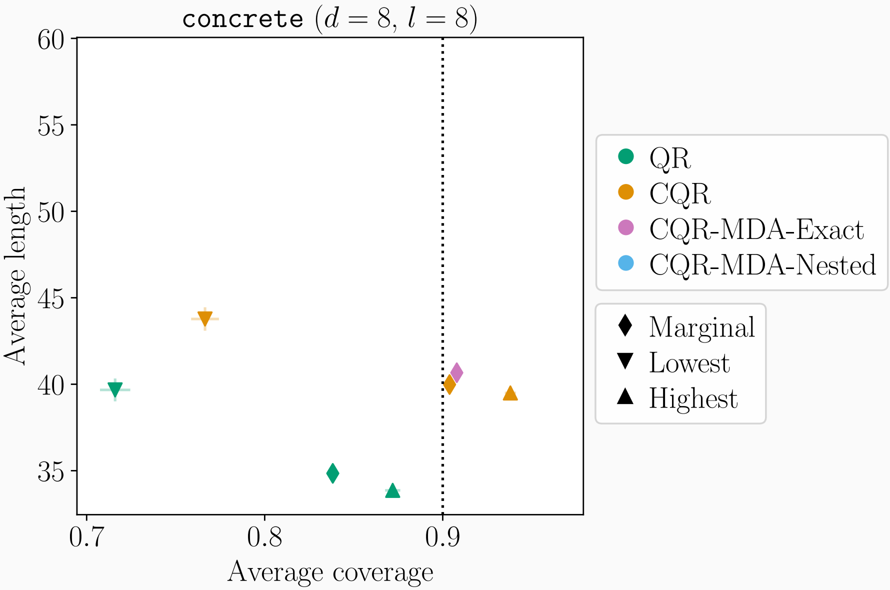
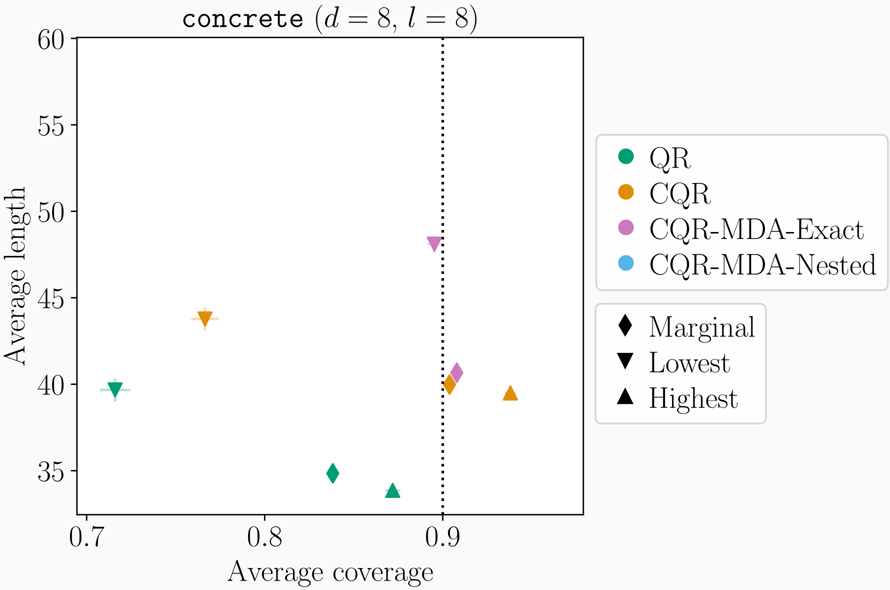
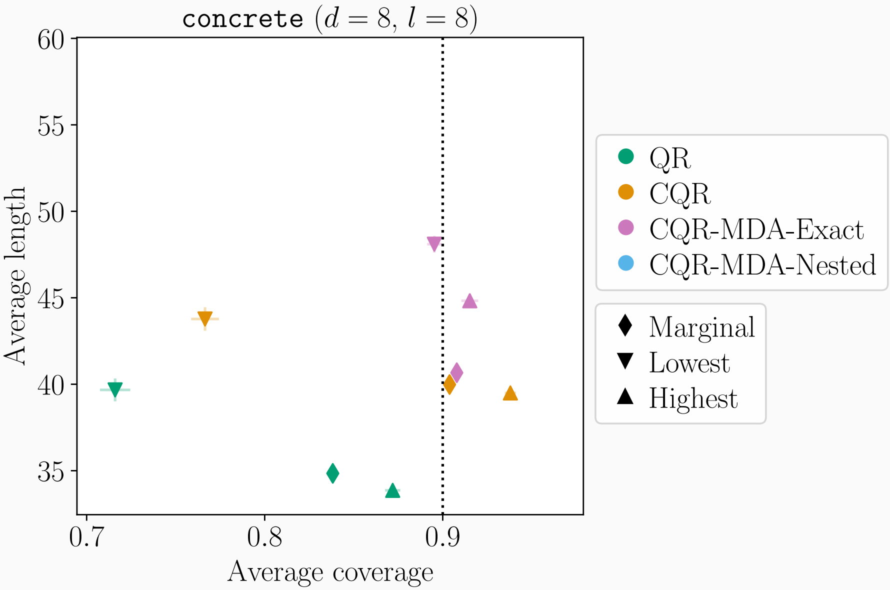



concrete ($d = 8$, $l = 8$)
60
55
50
45
40
35
Average length
0.7
0.8
0.9
Average coverage
QR
CQR
CQR-MDA-Exact
CQR-MDA-Nested
Marginal
Lowest
Highest

Semi-synthetic experiments



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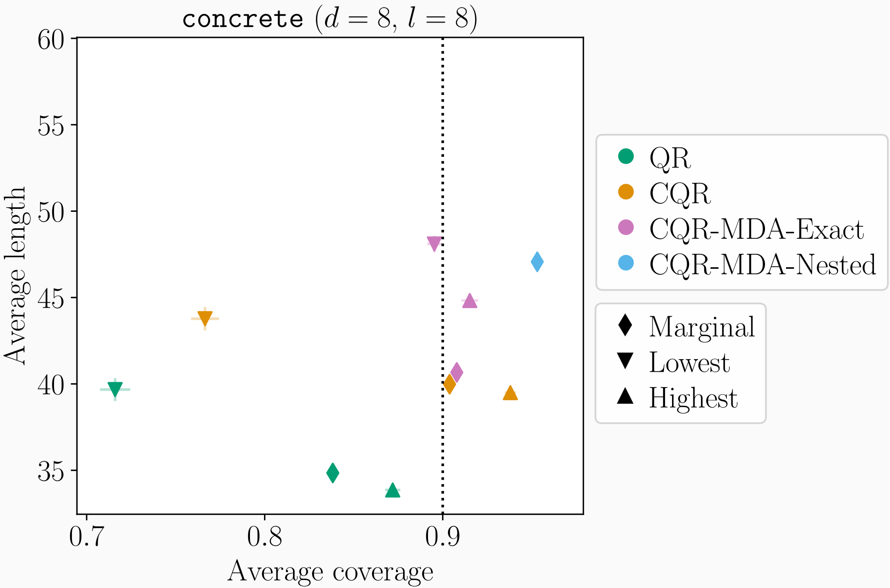

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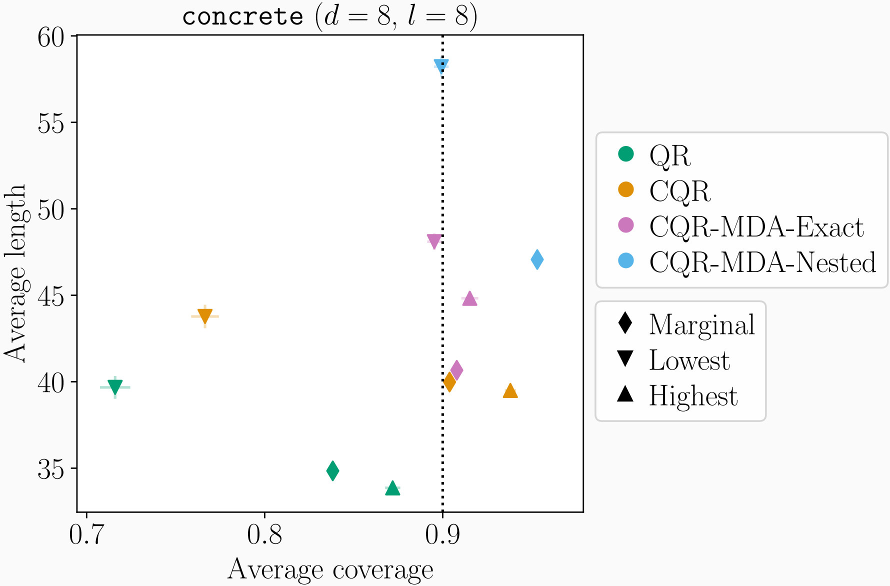

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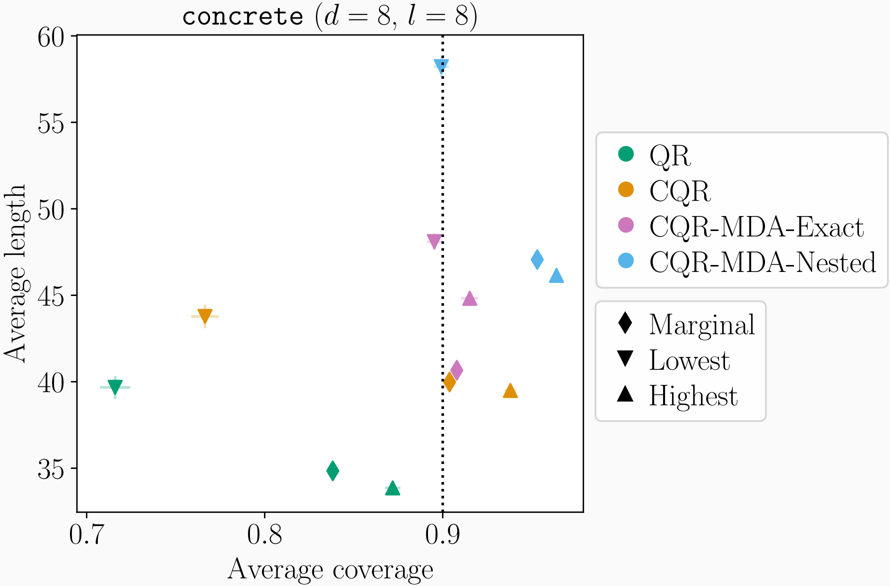
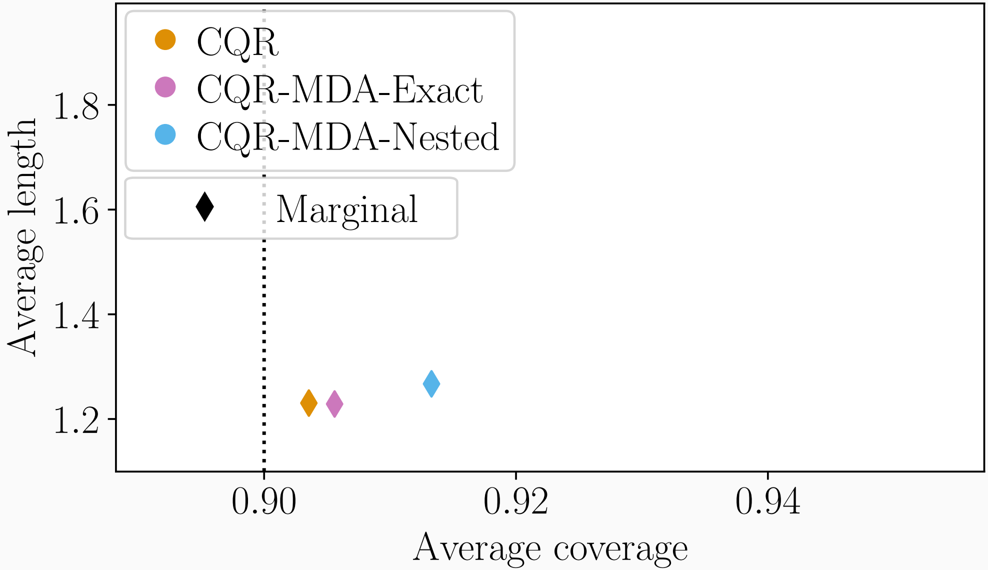
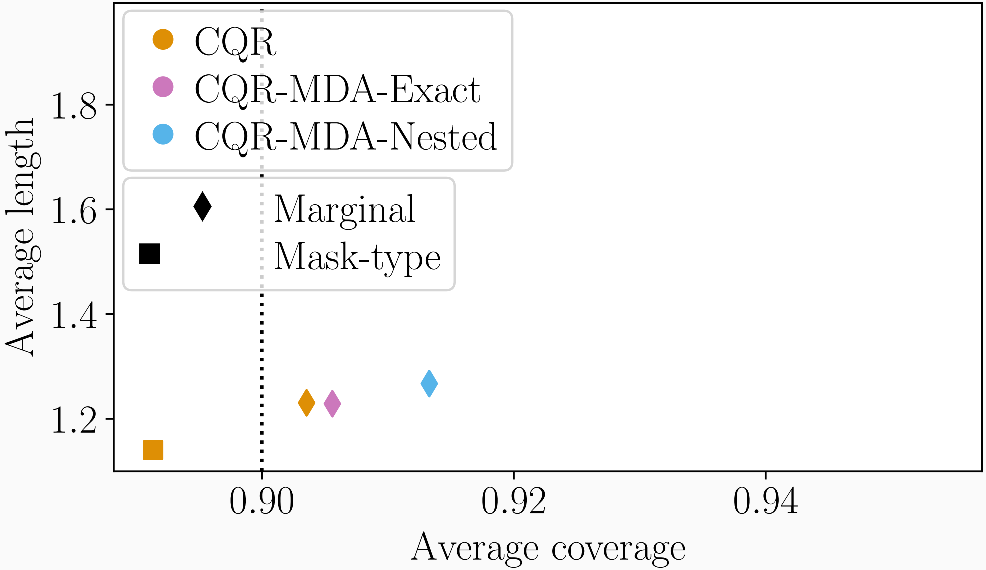
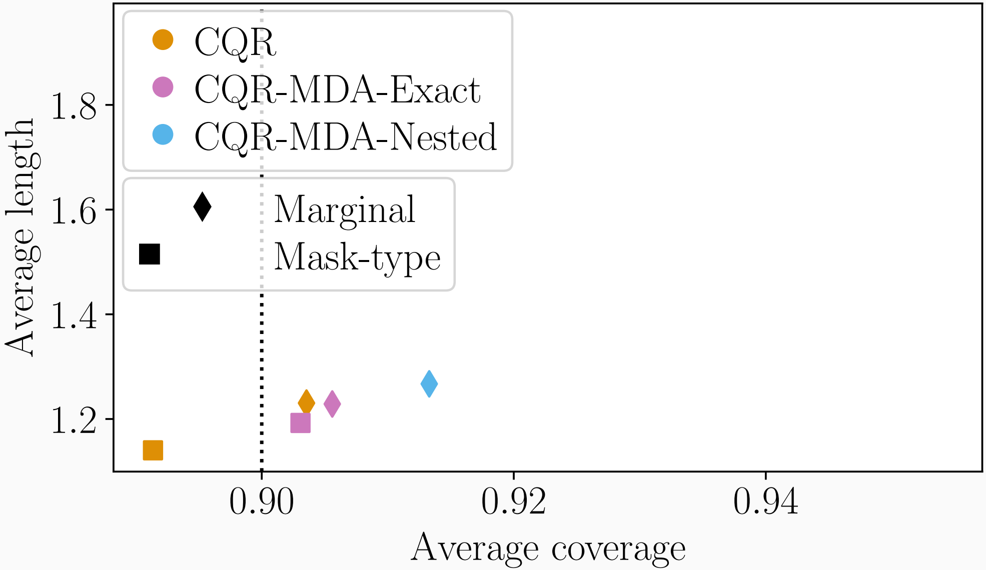




CQR
CQR-MDA-Exact
CQR-MDA-Nested
Marginal
Average length
1.8
1.6
1.4
1.2
0.90
0.92
0.94
Average coverage

Real data experiment: TraumaBase®, critical care medicine




CQR
CQR-MDA-Exact
CQR-MDA-Nested
Marginal
Mask-type
Average length
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1.4
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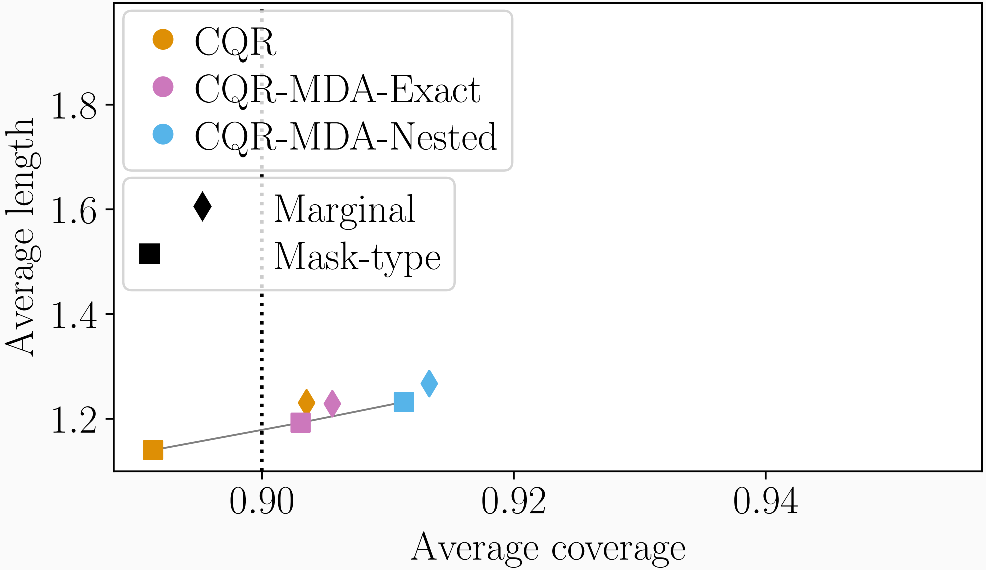
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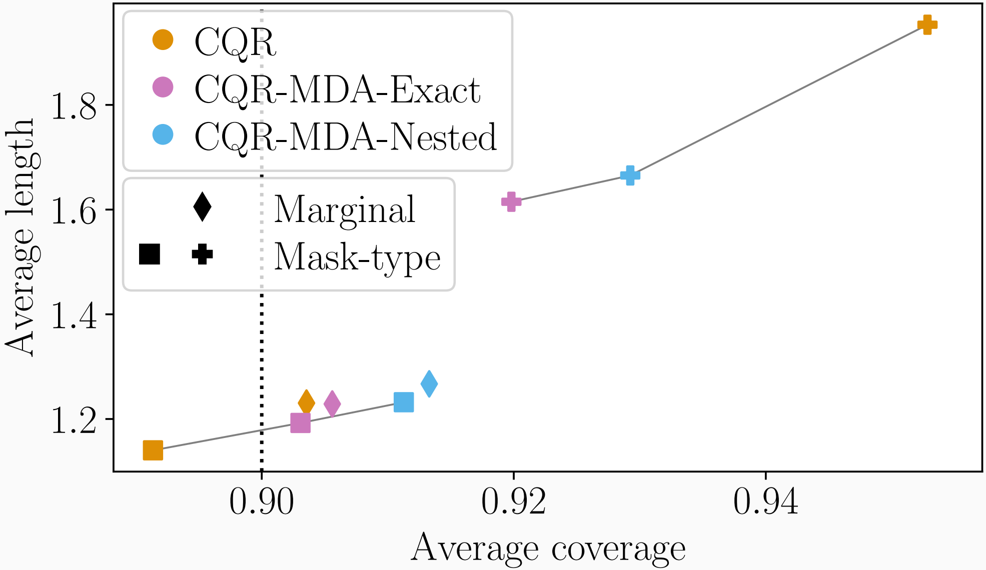

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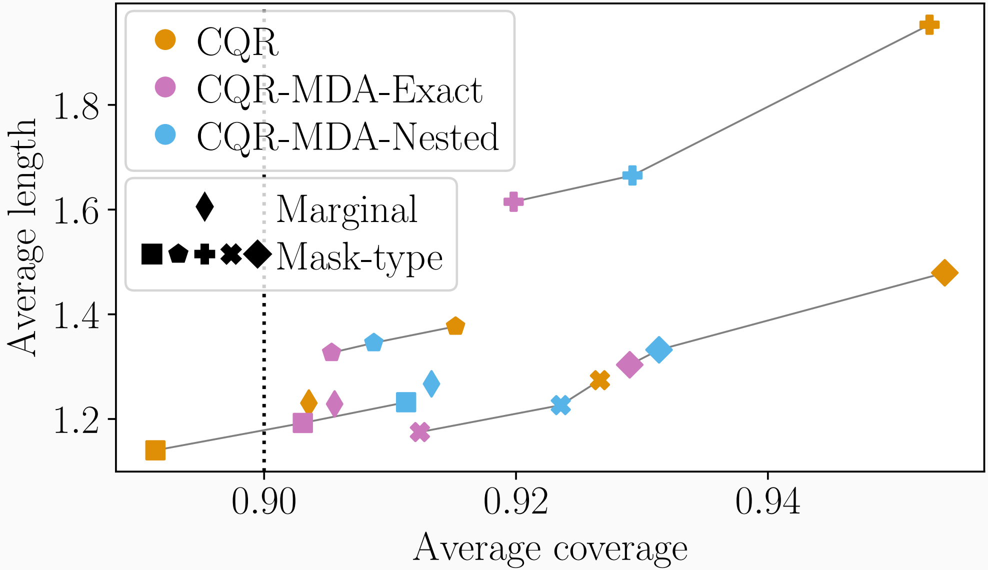

Introduction to missing values

Quantifying predictive uncertainty with missing values

Conclusion

Take-home-messages

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[11] *Conformal Prediction With Conditional Guarantees*

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[11] *Conformal Prediction With Conditional Guarantees*

Thank you! Questions? :)

References i

Ayme, A., Boyer, C., Dieuleveut, A., and Scornet, E. (2022). Near-optimal rate of consistency for linear models with missing values. *ICML*.

Barber, R. F., Candès, E. J., Ramdas, A., and Tibshirani, R. J. (2021). Predictive inference with the jackknife+. *The Annals of Statistics*, 49(1).

Gibbs, I., Cherian, J. J., and Candès, E. J. (2023). Conformal prediction with conditional guarantees.

Gupta, C., Kuchibhotla, A. K., and Ramdas, A. (2022). Nested conformal prediction and quantile out-of-bag ensemble methods. *Pattern Recognition*, 127.

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*.

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

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

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

Z. , M., Dieuleveut, A., Josse, J., and Romano, Y. (2023a). Conformal prediction with missing values. *ICML*.

Z. , M., Dieuleveut, A., Josse, J., and Romano, Y. (2023b). Predictive uncertainty quantification with missing values. To be submitted.

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

Appendix

Towards asymptotic individualized coverage

Consistency of a universal quantile learner after imputation

Let Φ be an imputation function chosen by the user.

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

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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.

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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 $\mathcal{C}^\infty$ 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.

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

$$d = 3$$

Data generation

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

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

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

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

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

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

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

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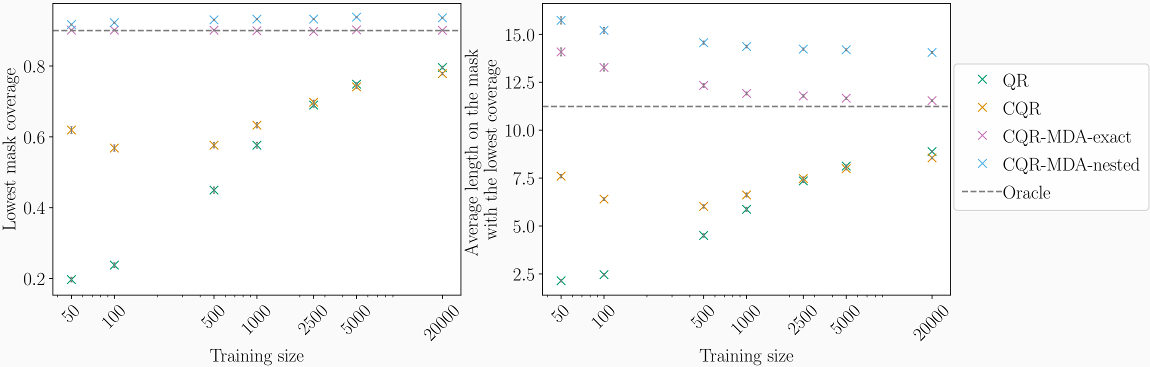
All components of X each have a probability 0.2 of being missing, Completely At Random.

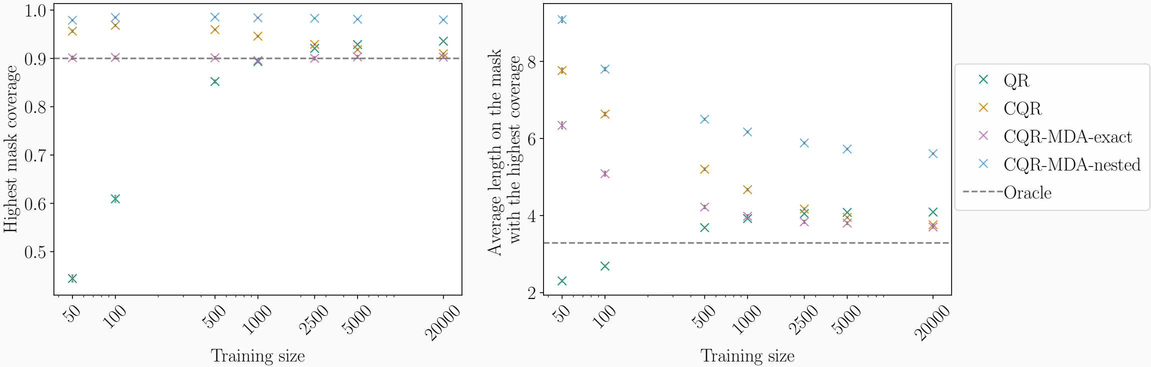
Simulation settings: varying training size

- 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

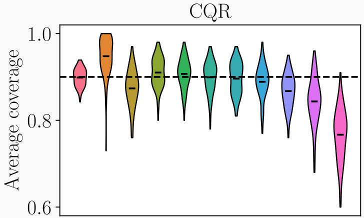
Results on the worst group



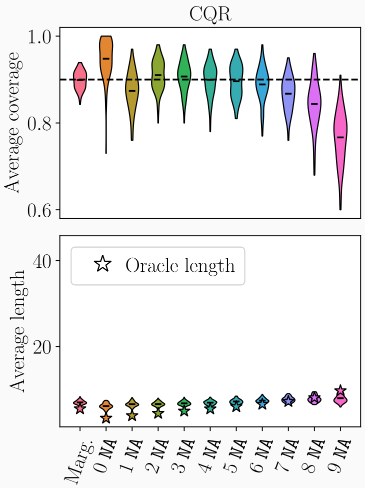
Results on the best group



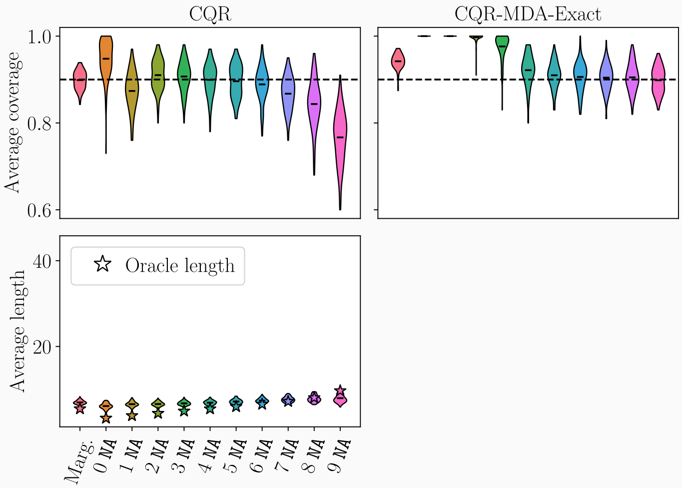
Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)



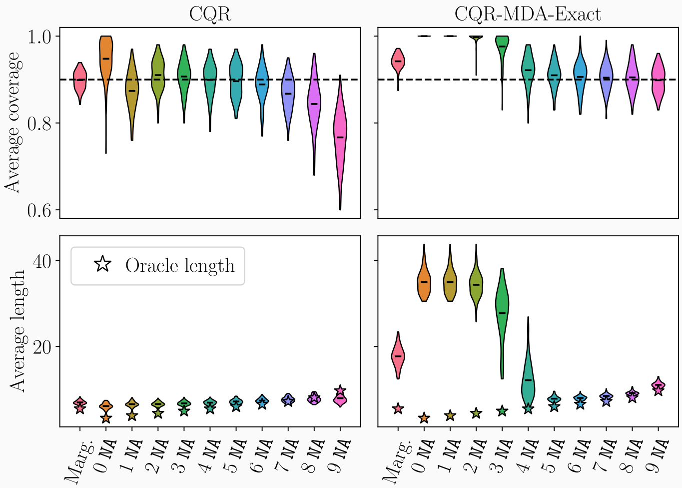
Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)



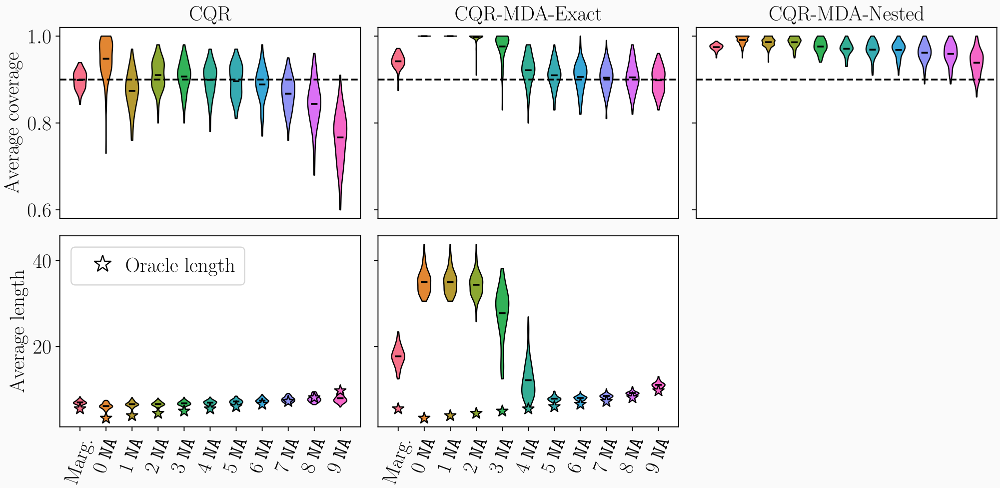
Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)



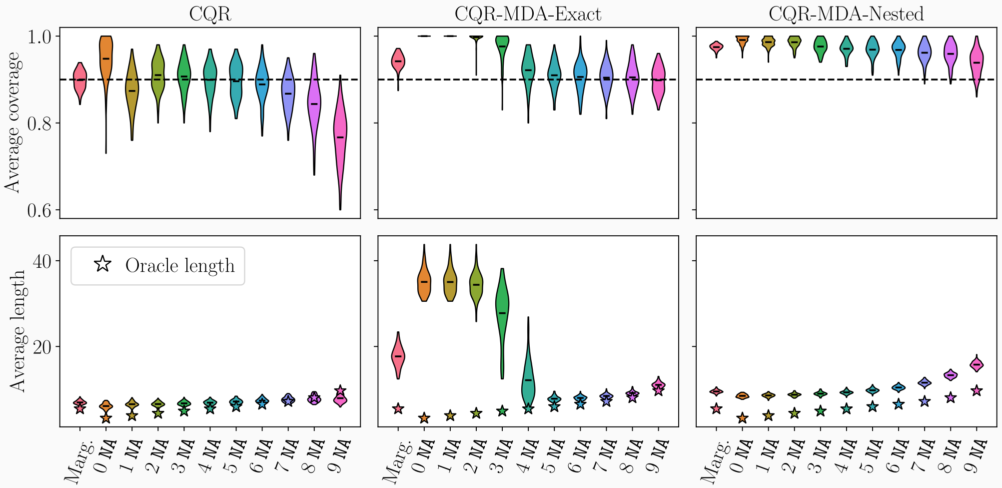
Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)



Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)



Synthetic experiments, 40% of missing values (Gaussian linear model, $d = 10$)

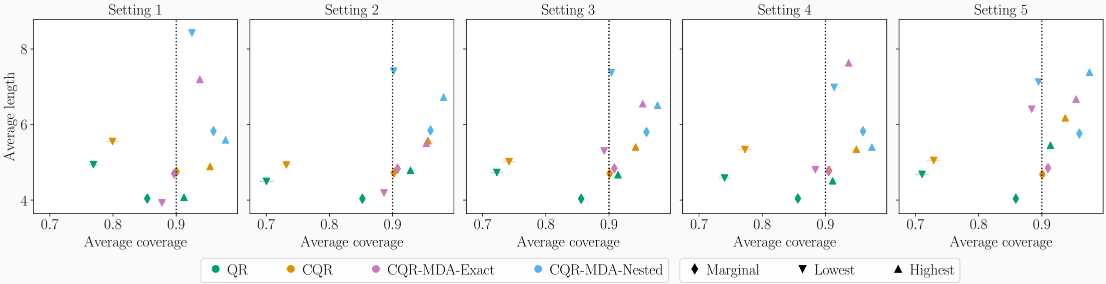


Simulation settings: beyond MCAR

- 6 variables (denote this set X_{missing}) out of 10 can be missing (the 4 others form the set X_{observed})
  $\rightarrow$ $X_{\text{missing}} = \{X_1, X_2, X_3, X_5, X_8, X_9\}$;
- Proportion of missing entries fixed to be 20%.

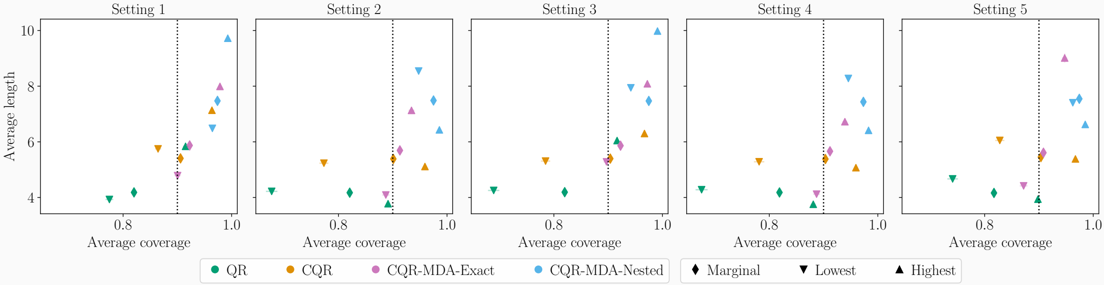
MAR missingness

- Probability of the variables in X_{missing} to be missing given by a logistic model of arguments X_{observed}.
- This setting is declined 5 times, with different weights for the logistic model.



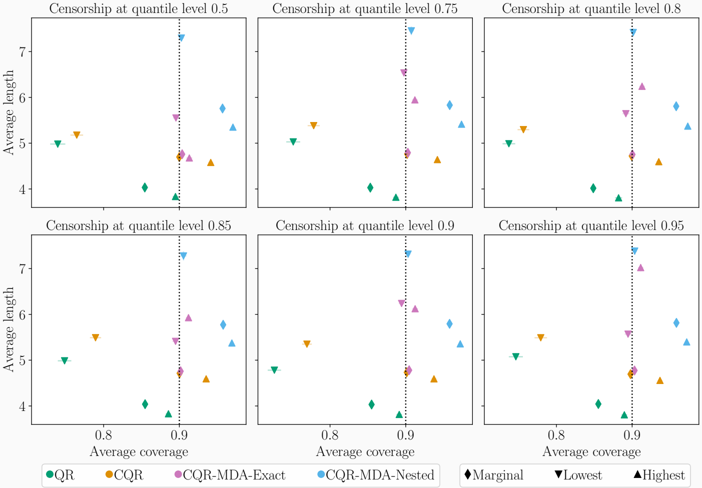
MNAR self masked missingness

- Probability of each variable in X_{missing} to be missing given by a logistic model of argument the same variable of X_{missing}.
- This setting is declined 5 times, with different weights for the logistic model.



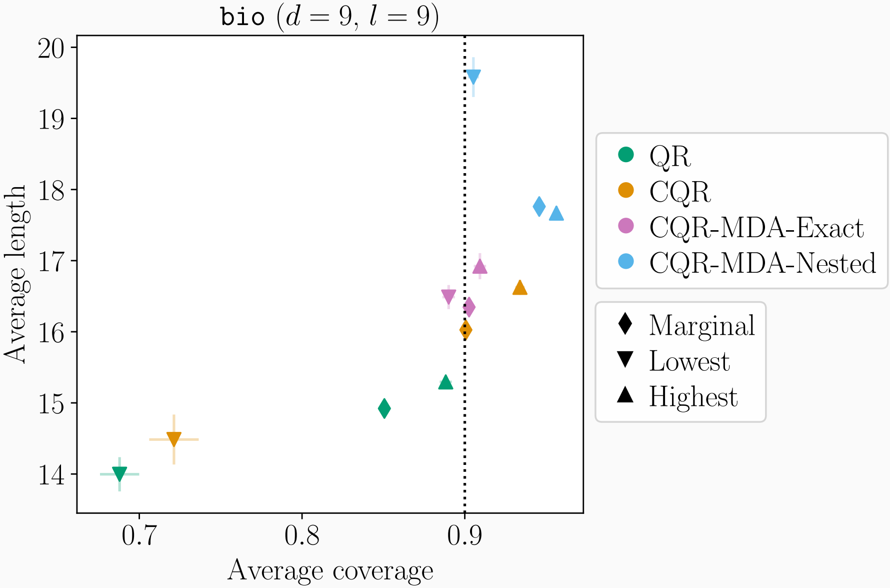
MNAR quantile censorship missingness

- Missing values are introduced at random in each q-quantile of the variables in X_{missing}.
- 6 different settings: q varies between 0.5, 0.75, 0.8, 0.85, 0.9 and 0.95.



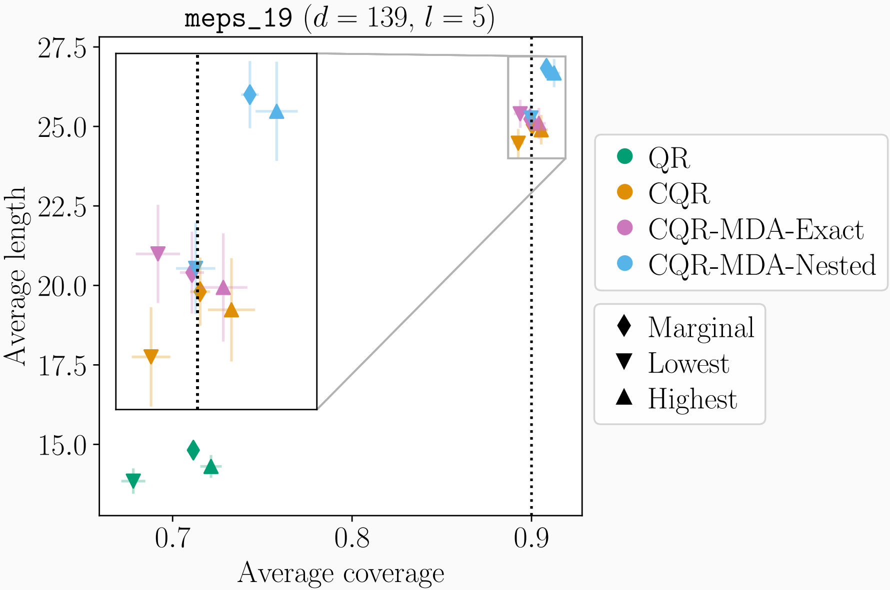
Semi-synthetic experiments

Bio data set

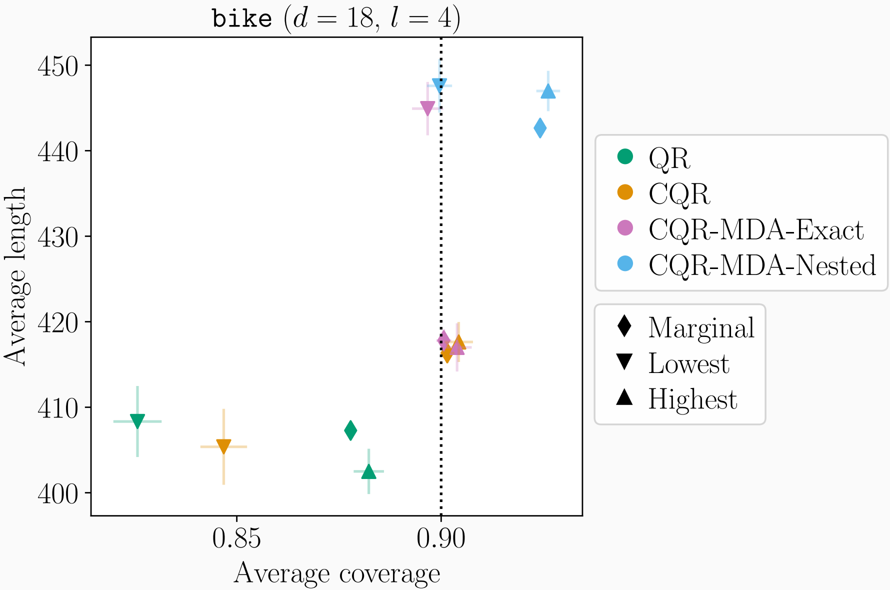


bio ($d = 9$, $l = 9$)
Average length
Average coverage
20
19
18
17
16
15
14
0.7
0.8
0.9
QR
CQR
CQR-MDA-Exact
CQR-MDA-Nested
Marginal
Lowest
Highest

`Meps_19` data set



Bike data set



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 $\mathsf{SI} = \frac{\mathsf{HR}}{\mathsf{SBP}}$, upon arrival at hospital (2.09% missing values);
- `HR`: the heart rate measured upon arrival of hospital (1.62% missing values).