NB: Open with an advanced pdf reader (e.g., Acrobat to have animations)

Lecture on Conformal Prediction

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ECAS-SFdS School

Previous lectures

1. On exchangeability (theory)
2. Split conformal prediction (methods) (theory)
3. Towards conditional coverage? (practical session) (theory) (case studies)
4. Beyond exchangeability (methods) (case studies)

Achievable definition of distribution-free validity

$\widehat{C}_\alpha$ = estimated predictive set based on n data points.

Definition (Distribution-free validity).

$\widehat{C}_\alpha$ achieves distribution-free validity if:

- for any distribution $\mathcal{D}$,
- for any associated exchangeable joint distribution $\mathcal{D}^{\mathrm{exch}(n+1)}$,

we have that:

$$\mathbb{P}_{\mathcal{D}^{\mathrm{exch}(n+1)}}\left(Y_{n+1} \in \widehat{C}_\alpha\left(X_{n+1}\right)\right) \geq 1 - \alpha.$$

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5. For a new point X_{n+1}, return

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

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

Split Conformal Prediction: summary

- **Simple** procedure which quantifies the uncertainty of **any** predictive model $\hat{A}$ by returning predictive regions
- **Finite-sample** guarantees
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$\hookrightarrow$ marginal also over the whole calibration set and the test point!

Calibration-condition coverage distribution under no tie

Theorem (Distribution conditional on the calibration data)**.**

If the scores are a.s. distinct, SCP outputs $\widehat{C}_\alpha$ such that for any distribution $\mathcal{D}$:

$$\mathbb{P}_{\mathcal{D}}\left(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1}) | (X_i, Y_i)_{i\in \mathrm{Cal}}\right) \sim \beta\left(k_\alpha, \#\mathrm{Cal} + 1 - k_\alpha\right),$$

with $k_\alpha = \lceil (1-\alpha)(\#\mathrm{Cal}+1) \rceil$.

From the β distribution, we get that it has

expectation $\dfrac{k_\alpha}{k_\alpha + \#\mathrm{Cal} + 1 - k_\alpha} = \dfrac{k_\alpha}{\#\mathrm{Cal}+1} = \dfrac{\lceil (1-\alpha)(\#\mathrm{Cal}+1) \rceil}{\#\mathrm{Cal}+1} \geq 1-\alpha$,

and variance $\dfrac{k_\alpha\left(\#\mathrm{Cal}+1-k_\alpha\right)}{\left(\#\mathrm{Cal}+1\right)^2\left(\#\mathrm{Cal}+2\right)} \approx \dfrac{\alpha(1-\alpha)}{\#\mathrm{Cal}+2}$.

SCP: what choices for the regression scores?

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

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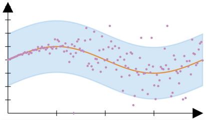
$$\widehat{C}_\alpha(X_{n+1}) = \{y \text{ such that } s\left(X_{n+1}, y; \hat{A}\right) \leq q_{1-\alpha}(\mathcal{S})\}$$

	Standard SCP Vovk et al. (2005)		
$s(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$		
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$		
Visu.			
✓	black-box around a "usable" prediction		
✗	not adaptive		

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	Standard SCP Vovk et al. (2005)		**CQR** Romano et al. (2019)
$s(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$		$\max(\widehat{\mathrm{QR}}_{\mathrm{lower}}(X) - Y, Y - \widehat{\mathrm{QR}}_{\mathrm{upper}}(X))$
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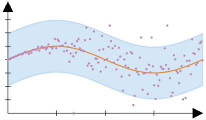
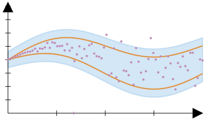
Visu.			
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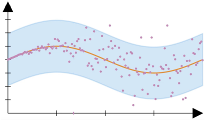
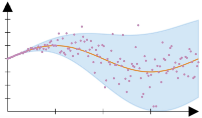
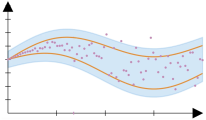
	Standard SCP Vovk et al. (2005)	**Locally weighted SCP** Lei et al. (2018)	**CQR** Romano et al. (2019)
$\mathrm{s}(\hat{A}(X), Y)$	$\lvert\hat{\mu}(X) - Y\rvert$	$\dfrac{\lvert\hat{\mu}(X) - Y\rvert}{\hat{\rho}(X)}$	$\max(\widehat{\mathrm{QR}}_{\text{lower}}(X) - Y, Y - \widehat{\mathrm{QR}}_{\text{upper}}(X))$
$\widehat{C}_\alpha(x)$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})]$	$[\hat{\mu}(x) \pm q_{1-\alpha}(\mathcal{S})\hat{\rho}(x)]$	$[\widehat{\mathrm{QR}}_{\text{lower}}(x) - q_{1-\alpha}(\mathcal{S}); \widehat{\mathrm{QR}}_{\text{upper}}(x) + q_{1-\alpha}(\mathcal{S})]$
Visu.			
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6. For a new point X_{n+1}, return

$$\widehat{C}_\alpha(X_{n+1}):=R_{q_{1-\alpha}(\mathcal{R})}\left(x;\hat{A}\right)=\left\{y\in\mathcal{Y}\text{ such that }\hat{r}\left(x,y\right)\leq q_{1-\alpha}\left(\mathcal{R}\right)\right\}$$

Some examples of nested sets (Gupta et al., 2022)

Example (Nested sets for the absolute value of the mean-regression residuals).

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Example (Nested sets for CQR).

$$\begin{aligned} & s\left(x, y; (\widehat{\mathrm{QR}}_{\mathrm{lower}}, \widehat{\mathrm{QR}}_{\mathrm{upper}})\right) \\ &= \max\left(\widehat{\mathrm{QR}}_{\mathrm{lower}}(x) - y, y - \widehat{\mathrm{QR}}_{\mathrm{upper}}(x)\right) \end{aligned} \quad \Longleftrightarrow \quad \begin{cases} R_t\left(\cdot; (\widehat{\mathrm{QR}}_{\mathrm{lower}}, \widehat{\mathrm{QR}}_{\mathrm{upper}})\right) \\ \equiv \left[\widehat{\mathrm{QR}}_{\mathrm{lower}}(\cdot) - t; \widehat{\mathrm{QR}}_{\mathrm{upper}}(\cdot) + t\right] \\ \mathcal{T} = \mathbb{R} \end{cases}$$

Where are we now?

1. On exchangeability (theory)
2. Split conformal prediction (methods) (theory) (practical session)
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Avoiding data splitting: full conformal and out-of-bags approaches

Full Conformal Prediction

Jackknife+

Handling missing data

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- lower statistical efficiency (lower model accuracy and higher predictive set size)
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Can we avoid splitting the data set?

The naive idea does not enjoy valid coverage (even empirically)

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✗ $\hat{A}$ obtained w. the training set $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ but not X_{n+1}.

Example ("Naive Idea" sets with an interpolating algorithm)**.**

Assume $\mathcal{A}$ interpolates:

- $\hat{A} = \mathcal{A}\left((x_1, y_1), \ldots, (x_n, y_n)\right)$
- $\hat{A}(x_k) - y_k = 0$ for any $k \in [\![1, n]\!]$

$\Rightarrow$ Naive method above *(with MAE score functions)* outputs $\{\hat{A}\left(X_{n+1}\right)\}$ (a single point) for any new test point!

Full Conformal Prediction[9] does not discard training points!

- Full *(or transductive)* Conformal Prediction
  - avoids data splitting

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

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- **Idea**: the most probable labels Y_{n+1} live in $\mathcal{Y}$, and have a low enough conformity score. By looping over all possible $y \in \mathcal{Y}$, the ones leading to the smallest conformity scores will be found.

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Full Conformal Prediction (CP): recovering exchangeability

For any candidate (X_{n+1}, y):

1. Get $\hat{A}_y$ by training $\mathcal{A}$ on $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \cup \{(X_{n+1}, y)\}$

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2. Obtain a set of training scores
$$\mathcal{S}_y^{(\text{train})} = \left\{ \mathsf{s}(\hat{A}_y(X_i), Y_i) \right\}_{i=1}^{n} \cup \{ \mathsf{s}(\hat{A}_y(X_{n+1}), y)\}$$
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- ✓ Test point treated in the same way than train points
- ✓ Any score works
- ✗ Computationally costly

Definition (Symmetrical algorithm).

A deterministic algorithm $\mathcal{A} : (U_1, \ldots, U_n) \mapsto \hat{A}$ is symmetric if for any permutation σ of $[\![1, n]\!]$: $\mathcal{A}(U_1, \ldots, U_n) \overset{\text{a.s.}}{=} \mathcal{A}\left(U_{\sigma(1)}, \ldots, U_{\sigma(n)}\right)$.

Full CP: theoretical foundation

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If the algorithm $\mathcal{A} : (U_1, \ldots, U_n) \mapsto \hat{A}$ is symmetric, and $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable, then $S_1, \ldots, S_{n+1}$ are exchangeable, with

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Moreover

$$\begin{aligned}
Y_{n+1} \in \widehat{C}_\alpha^{\text{Full}}(X_{n+1}) &:= \left\{ y \text{ such that } \boxed{\mathrm{s}} \left(\hat{A}_y \left(X_{n+1} \right), y \right) \leq q_{1-\alpha} \left(\mathcal{S}_y^{(\text{train})} \right) \right\} \\
&\Leftrightarrow \boxed{\mathrm{s}} \left(\hat{A}_{Y_{n+1}} \left(X_{n+1} \right), Y_{n+1} \right) \leq q_{1-\alpha} \left(\mathcal{S}_{Y_{n+1}}^{(\text{train})} \right) \\
&\Leftrightarrow S_{n+1} \leq q_{1-\alpha}(S_1, \ldots, S_n, S_{n+1}) \; !
\end{aligned}$$

Full CP: theoretical guarantees

Full CP enjoys finite sample guarantees proved in Vovk et al. (2005).

Theorem (Marginal validity of Full CP Vovk et al. (2005)).

Suppose that

(i) $(X_i, Y_i)_{i=1}^{n+1}$ are exchangeable,

(ii) the algorithm $\mathcal{A}$ is symmetric.

Full CP applied on $(X_i, Y_i)_{i=1}^{n} \cup \{X_{n+1}\}$ outputs $\widehat{C}_\alpha(\cdot)$ such that:

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

Additionally, if the scores are a.s. distinct:

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

Interpolation regime

Example (FCP sets with an interpolating algorithm)**.**

Assume $\mathcal{A}$ interpolates:

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$\Rightarrow$ Full Conformal Prediction *(with standard score functions)* outputs $\mathcal{Y}$ (the whole label space) for any new test point!

Split Conformal Prediction is a special case of Full Conformal Prediction

- Set $\hat{A}_y \equiv \hat{A}$, constant, independent of $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \cup \{(X_{n+1}, y)\}$
- Then, running Full Conformal Prediction corresponds to Split Conformal Prediction with $\#\mathrm{Cal} = n$.

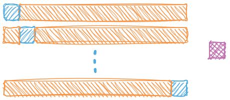
Avoiding data splitting: full conformal and out-of-bags approaches

Full Conformal Prediction

Jackknife+

Handling missing data

Jackknife: the naive idea does not enjoy valid coverage



- Based on leave-one-out (LOO) residuals
- $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ training data
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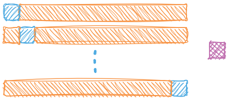

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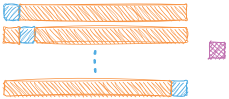

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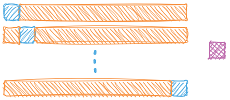

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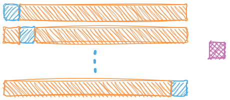

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Warning

No guarantee on the prediction of $\hat{A}$ with scores based on $(\hat{A}_{-i})_i$, without assuming a form of **stability** on $\mathcal{A}$.

Jackknife+ (Barber et al., 2021)

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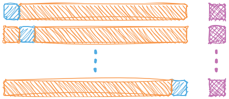

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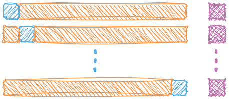

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(in standard mean regression)

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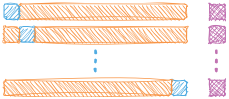

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Recall $q_{\beta,\inf}(X_1, \ldots, X_n) := \lfloor \beta \times n \rfloor$ smallest value of $(X_1, \ldots, X_n)$

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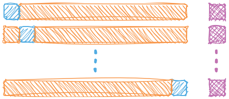

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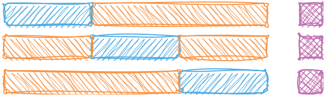
CV+ Barber et al. (2021) (see also cross-conformal predictors: Vovk, 2015)



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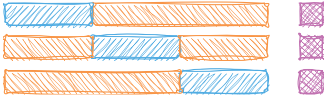

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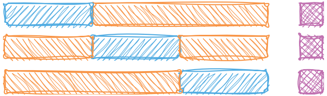
$$\mathcal{S}_{\text{up/down}} = \left\{ \left\{ \hat{A}_{-F_k}(X_{n+1}) \pm \left| \hat{A}_{-F_k}(X_i) - Y_i \right| \right\}_{i \in F_k} \right\}_k \cup \{\pm\infty\}$$

(in standard mean regression)

CV+ Barber et al. (2021) (see also cross-conformal predictors: Vovk, 2015)



- Based on cross-validation residuals
- $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ training data
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- Build the predictive interval: $[q_{\alpha,\inf}(\mathcal{S}_{\text{down}}); q_{1-\alpha}(\mathcal{S}_{\text{up}})]$

Recall $q_{\beta,\inf}(X_1, \dots, X_n) := \lfloor \beta \times n \rfloor$ smallest value of $(X_1, \dots, X_n)$

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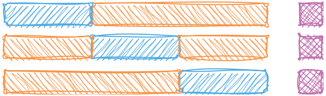

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Theorem (Marginal validity of CV+ Barber et al. (2021)).

If $\mathcal{D}_n \cup (X_{n+1}, Y_{n+1})$ are exchangeable and $\mathcal{A}$ is symmetric: $\mathbb{P}(Y_{n+1} \in \widehat{C}_\alpha(X_{n+1})) \geq 1 - 2\alpha - \min\left(\frac{2(1-1/K)}{n/K+1}, \frac{1-K/n}{K+1}\right) \geq 1 - 2\alpha - \sqrt{2/n}$.

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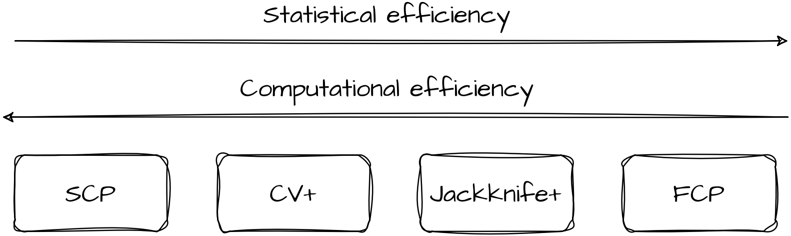
General overview



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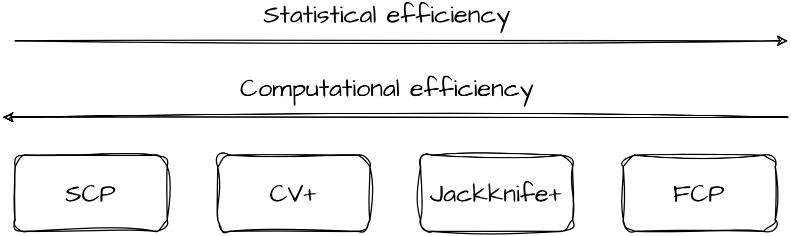

- Generalized framework encapsulating out-of-sample methods: Nested CP (Gupta et al., 2022) $\rightarrow$ extends *JK+/CV+ for any score.*

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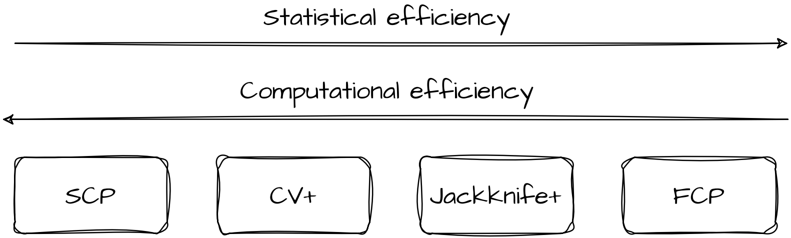

- Generalized framework encapsulating out-of-sample methods: Nested CP (Gupta et al., 2022) $\rightarrow$ extends *JK+/CV+ for any score.*
- Accelerating FCP: Nouretdinov et al. (2001); Lei (2019); Ndiaye and Takeuchi (2019); Cherubin et al. (2021); Ndiaye and Takeuchi (2022); Ndiaye (2022)

Non exhaustive references.

Avoiding data splitting: full conformal and out-of-bags approaches

Handling missing data

- Supervised learning setting with missing covariates
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- Is MCV a too lofty goal?!
- Achieving MCV under $M \perp\!\!\!\perp X$ and $Y \perp\!\!\!\perp M \mid X$
- Experimental results

A collaboration

Yaniv Romano

Technion - Israel Institute of Technology

Julie Josse

PreMeDICaL

INRIA

Aymeric Dieuleveut

École Polytechnique

- *Predictive Uncertainty Quantification with Missing Covariates*, 2024
- *Conformal Prediction with Missing Values*, ICML 2023

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 are ubiquitous and challenging

Data: $\left(X^{(k)}, \qquad Y^{(k)}\right)_{k=1}^{n}$

Y	X_1	X_2	X_3
22	5	6	3
19	6	8	NA
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If each entry has a probability 0.01 of being missing:

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

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

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$\Rightarrow$ Statistical and computational challenges.

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Supervised learning with missing values: impute-then-predict

Impute-then-predict procedures are widely used.

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\begin{array}{c}
x^{(1)} \\ x^{(2)} \\ x^{(3)} \\ x^{(4)}
\end{array}
\begin{bmatrix}
-1 & -10 & 6 & 0 \\
4 & \texttt{NA} & -2 & 2 \\
5 & 1 & 2 & \texttt{NA} \\
0 & \texttt{NA} & \texttt{NA} & 1
\end{bmatrix}
\xrightarrow{\quad \phi \quad}
\begin{array}{c}
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\end{array}
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2. Train your algorithm (Random Forest, Neural Nets, etc.) on the imputed data:

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

Supervised learning with missing values: impute-then-predict, cont'd

✓ Le Morvan et al. (2021)[2] show that for **any deterministic imputation** and **universal learner** this procedure is **Bayes-consistent**.

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Supervised learning with missing values: impute-then-predict, cont'd

- ✓ Le Morvan et al. (2021)[2] show that for any deterministic imputation and universal learner this procedure is Bayes-consistent.
- ✗ Ayme et al. (2022)[3] show that even for very **simple distributions** (linear model, Gaussian noise), this rate of convergence may suffer from **curse of dimensionality**.

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

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

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- Goals and challenges for predictive uncertainty quantification
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Goals of 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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Definition (1. Marginal Validity (MV)).

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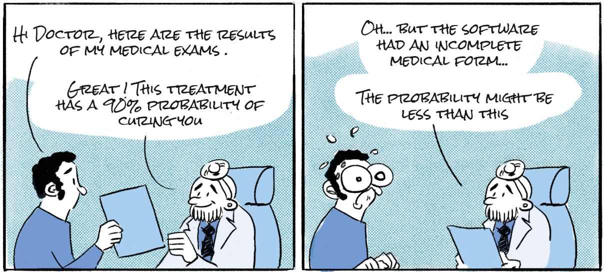
Definition (2. Mask-Conditional-Validity (MCV)).

$$\mathbb{P}\left\{Y^{(n+1)} \in \mathcal{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right) | M^{(n+1)}\right\} \overset{a.s.}{\geq} 1-\alpha. \tag{MCV}$$



Illustrations @theoremlinger

CP is marginally valid (MV) after imputation

Lemma (Exchangeability after imputation (Z., Dieuleveut, Josse and Romano, 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:
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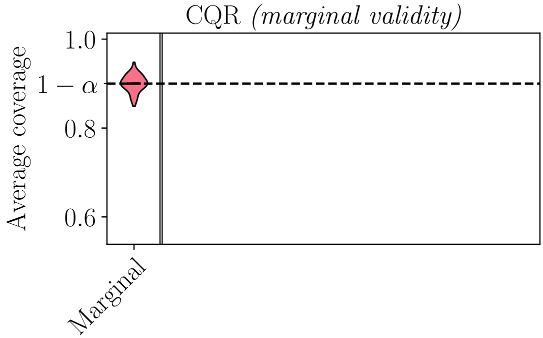
CP is marginally valid on imputed data sets

$Y = \beta^T X + \varepsilon$, $\beta = (1, 2, -1)^T$, X and ε Gaussian.



✓ Marginal (i.e. average) coverage (MV) is indeed recovered!

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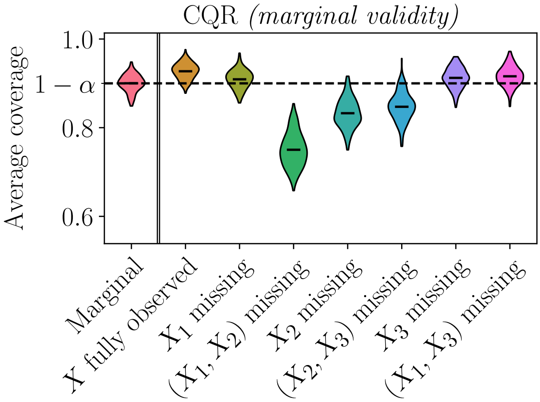
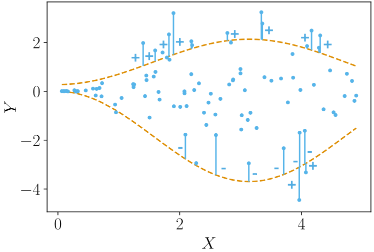


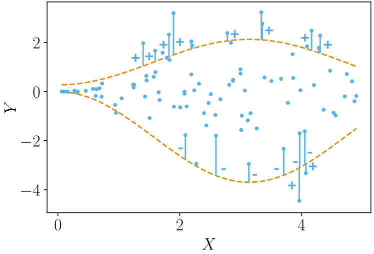
- ✓ Marginal (i.e. average) coverage (MV) is indeed recovered!
- ✗ Mask-conditional-validity (MCV) is not attained
  - ↪ Missing values induce heteroskedasticity
    (supported by theory under (non-)parametric assumptions)

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!

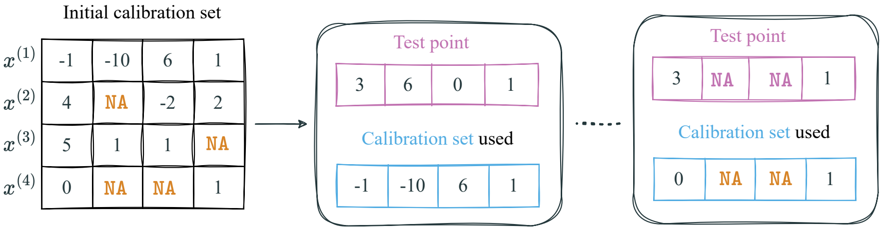


Observation: the α-correction term is computed among all the data points, regardless of their mask!



Warning: 2^d possible masks

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



Conceptually: a structured distribution shift situation

1. For each pattern m, we have a different distribution for $(X_{\mathrm{obs(M)}}, Y)|M = m$.

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Conceptually: a structured distribution shift situation

1. For each pattern m, we have a different distribution for $(X_{\mathrm{obs(M)}}, Y)|M = m$.
2. Those distributions are connected.
3. Reasonable model of the link between pattern and the uncertainty.

Fully distribution-free MCV is necessarily uninformative

Theorem (General MCV hardness result (Z., Josse, Romano and Dieuleveut, 2024)[4]).

If any $\widehat{C}_\alpha$ is distribution-free MCV then for any distribution P, for any mask m such that $P_M(m) > 0$, it holds:

$$\mathbb{P}_{P^{\otimes(n+1)}}\left(\text{mes}\left(\widehat{C}_\alpha\left(X_{n+1}, m\right)\right) = \infty\right) \geq 1 - \alpha - \Delta_{m,n} \geq 1 - \alpha - P_M(m)\sqrt{n+1}.$$

[4] An analogous statement is also available for the classification framework.

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Irreducible term: consider $\widehat{C}_\alpha$ outputting $\mathcal{Y}$ with probability $1 - \alpha$ and $\emptyset$ otherwise.

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$\Delta_{m,n}$ term: smaller than $P_M(m)\sqrt{n+1}$

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Irreducible term: consider $\widehat{C}_\alpha$ outputting $\mathcal{Y}$ with probability $1 - \alpha$ and $\emptyset$ otherwise.

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$\hookrightarrow$ gets negligible (making the lower bound nearly $1 - \alpha$) for low probability masks compared to n;

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Irreducible term: consider $\widehat{C}_\alpha$ outputting $\mathcal{Y}$ with probability $1-\alpha$ and $\emptyset$ otherwise.

$\Delta_{m,n}$ term: smaller than $P_M(m)\sqrt{n+1}$

- $\hookrightarrow$ gets negligible (making the lower bound nearly $1-\alpha$) for low probability masks compared to n;
- $\hookrightarrow$ gets large (making the lower bound trivial because negative) for high probability masks compared to n.

[4] An analogous statement is also available for the classification framework.

Restricting the link between M and $(X \text{or} Y)$ does not allow informative MCV

Analogous statements are also available for the classification framework.

Restricting the link between M and $(X \text{or} Y)$ does not allow informative MCV

Theorem ($M \perp\!\!\!\perp X$ hardness result (Z., Josse, Romano and Dieuleveut, 2024)).

If any $\widehat{C}_\alpha$ is MCV under $M \perp\!\!\!\perp X$, then for any distribution P such that $M \perp\!\!\!\perp X$, for any mask m such that $P_M(m) > 0$, it holds:

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Theorem ($Y \perp\!\!\!\perp M \mid X$ hardness result (Z., Josse, Romano and Dieuleveut, 2024)).

If any $\widehat{C}_\alpha$ is MCV under $Y \perp\!\!\!\perp M \mid X$, then for any distribution P such that $Y \perp\!\!\!\perp M \mid X$, for any mask m such that $\frac{1}{\sqrt{2}} \geq P_M(m) > 0$, it holds:

$$\mathbb{P}_{P^{\otimes(n+1)}}\left(\text{mes}\left(\widehat{C}_\alpha\left(X_{n+1}, m\right)\right) = \infty\right) \geq 1 - \alpha - \Delta_{m,n} \geq 1 - \alpha - 2P_M(m)\sqrt{n+1}.$$

Analogous statements are also available for the classification framework.

Restricting the link between M and $(X \text{or} Y)$ does not allow informative MCV

Theorem ($M \perp\!\!\!\perp X$ hardness result (Z., Josse, Romano and Dieuleveut, 2024)).

If any $\widehat{C}_\alpha$ is MCV under $M \perp\!\!\!\perp X$, then for any distribution P such that $M \perp\!\!\!\perp X$, for any mask m such that $P_M(m) > 0$, it holds:

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$\Rightarrow$ need to restrict both the link between M and X, as well as between M and Y.

Analogous statements are also available for the classification framework.

Missing Data Augmentation (MDA) of the calibration set

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

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
$\tilde{x}^{(3)}$	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

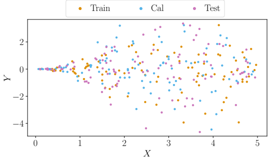
Calibration set used

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

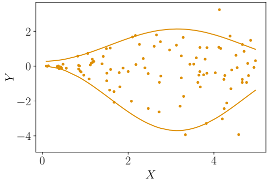
$\#\mathrm{Cal}^{\mathrm{M}^{(\text{test})}}$ observations

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

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

3	NA	NA	1

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

5.1 For each $j \in [\![1, d]\!]$ s.t. $M_j^{(n+1)} = 1$, set $\tilde{M}_j^{(k)} = 1$ 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`
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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
$\tilde{x}^{(3)}$				
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CQR-MDA with exact masking in words

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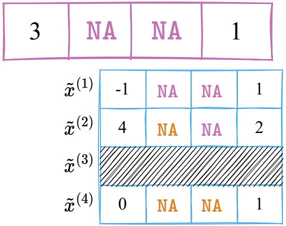
   5.2 Impute the new calibration set

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



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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

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
4. Train the quantile regressors on the imputed proper training set
5. For a test point $\left(X^{(n+1)}, M^{(n+1)}\right)$:

3	NA	NA	1

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

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

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

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)[5] and Gupta et al. (2022)[6].

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

[6] *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 $\left(X^{(n+1)}, M^{(n+1)}\right)$:

    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:

        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

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

3	NA	NA	1

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

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

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 $\widehat{QR}_{1-\alpha/2}(\tilde{X}^{(n+1),k})$

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 $q_{1-\alpha}(\{Z^{(k)}_{\text{upper}}\}_{k\in\mathrm{Cal}})$

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

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)**.**

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

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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

CP-MDA-Nested* (Missing Data Augmentation)

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

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Overmasked calibration set

Test point

3	NA	NA	1	2

Initial calibration set

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

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

$i)$ keep same mask

Overmasked calibration set

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

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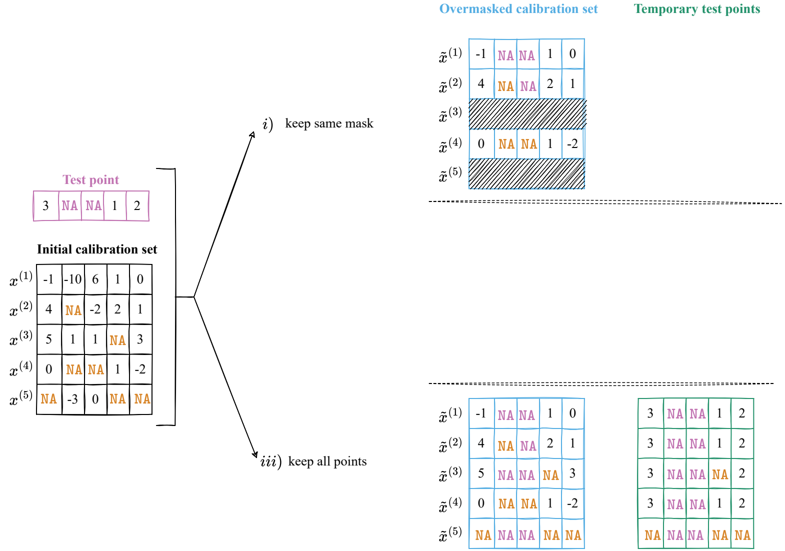

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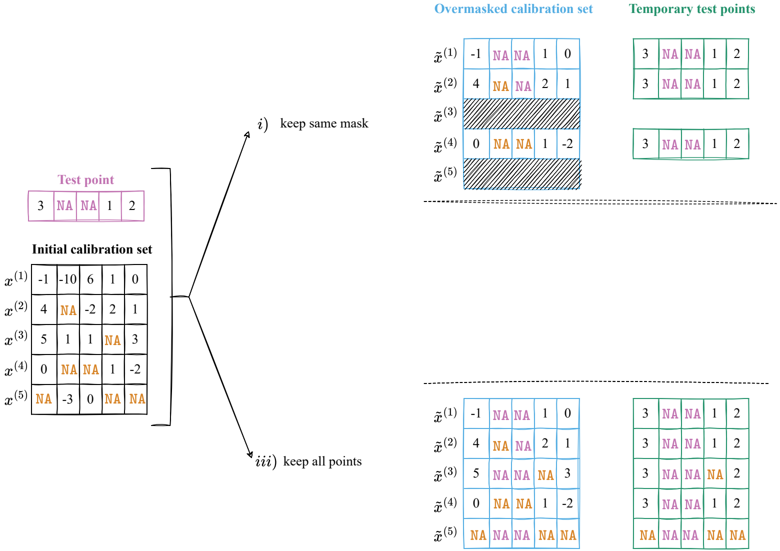

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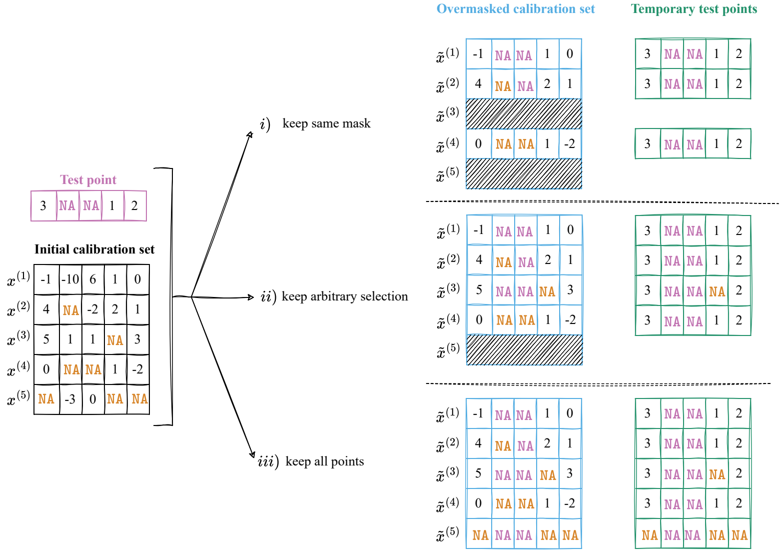
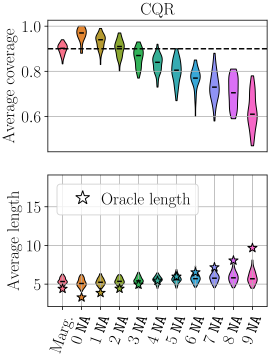


Experiments on $M \perp\!\!\!\perp X$ and $Y \perp\!\!\!\perp M \mid X$ Gaussian linear data in dimension 10



20% of missing values

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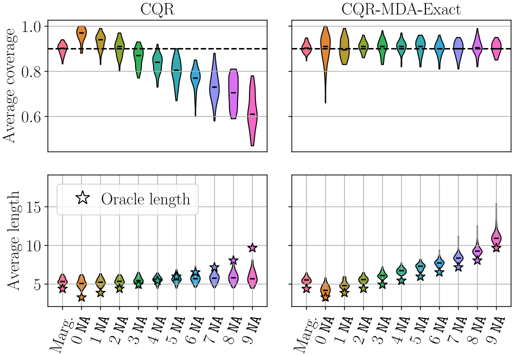

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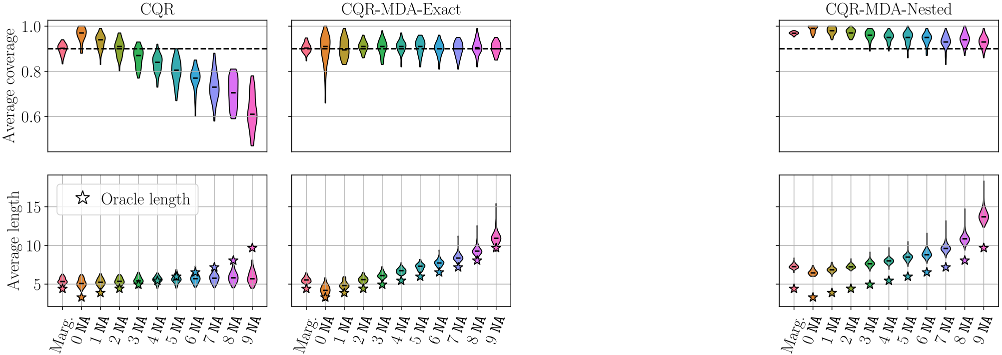

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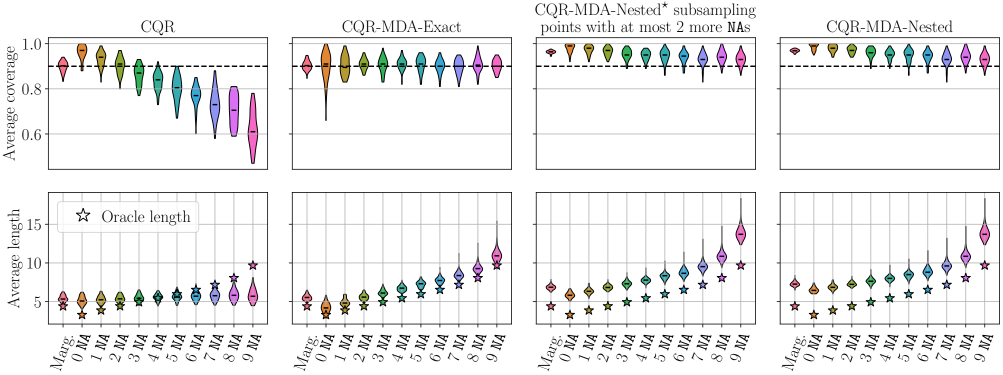

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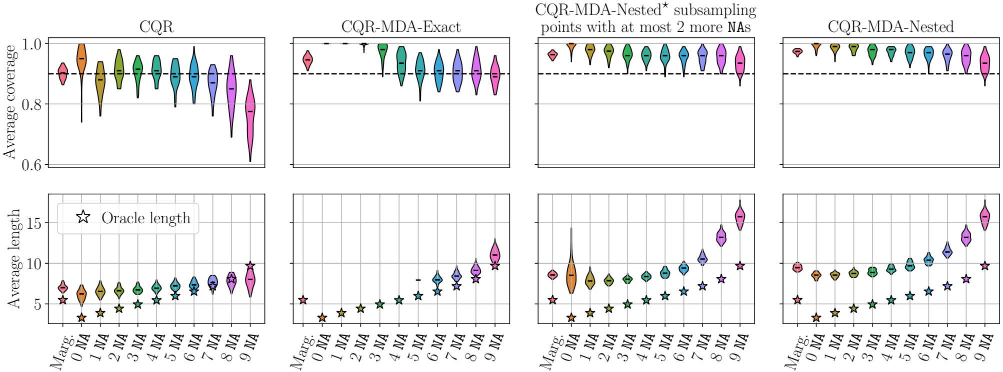

40% of missing values

Theorem (Mask-conditional-validity of CP-MDA-Nested* (Z., Josse, Romano and Dieuleveut, 2024)).

Under the assumptions that:

- $M \perp\!\!\!\perp (X, Y)$,
- $\left(X^{(k)}, M^{(k)}, Y^{(k)}\right)_{k=1}^{n+1}$ are i.i.d.,

then, for almost all imputation function, CP-MDA-Nested* reaches (MCV) at the level $1 - 2\alpha$, that is:

$$\mathbb{P}\left\{Y^{(n+1)} \in \widehat{C}_\alpha\left(X^{(n+1)}, M^{(n+1)}\right) | M^{(n+1)}\right\} \overset{a.s.}{\geq} 1 - 2\alpha.$$

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Proof elements:

1. Crop the data sets to hide the missing entries of the test point
2. Applying the mask of the calibration point corresponds to a predictor that draws a predictions randomly

$\Rightarrow$ Use the same proof arguments than (Barber et al., 2021) on random predictors

Valididities of 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:

Definition (1. Marginal Validity (MV)).

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	Exisiting approaches	
(MV)	✓ (Z., Dieuleveut, Josse, and Romano, 2023)	
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(MV)	✓ (Z., Dieuleveut, Josse, and Romano, 2023)	✓
(MCV)	✗	✓

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(MCV)	✗	✓ under $M \perp\!\!\!\perp (X, Y)$

Some settings

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

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- **Concatenate the mask in the features**
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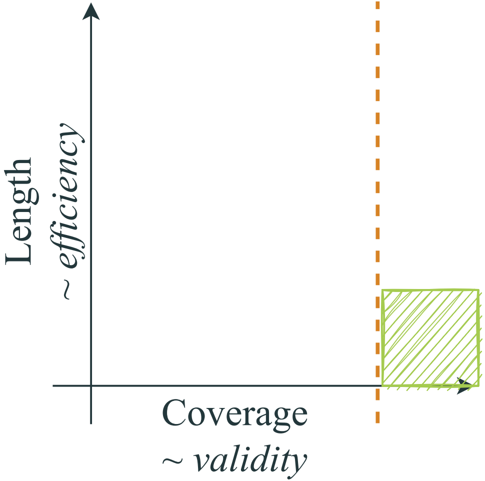
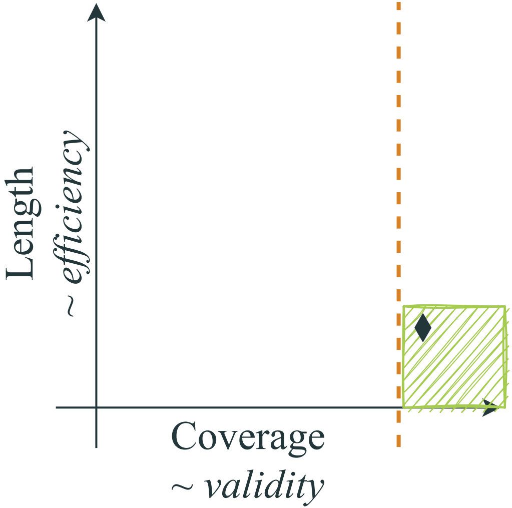
- (Semi)-synthetic experiments:
  - Uniform MCAR missing values, with probability 20%
  - 100 repetitions


Length
$\sim$ *efficiency*
Coverage
$\sim$ *validity*

Before more experiments, visualisation



♦ : marginal coverage, i.e.

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

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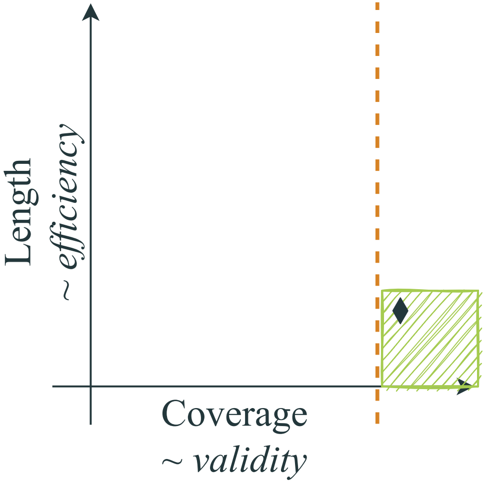

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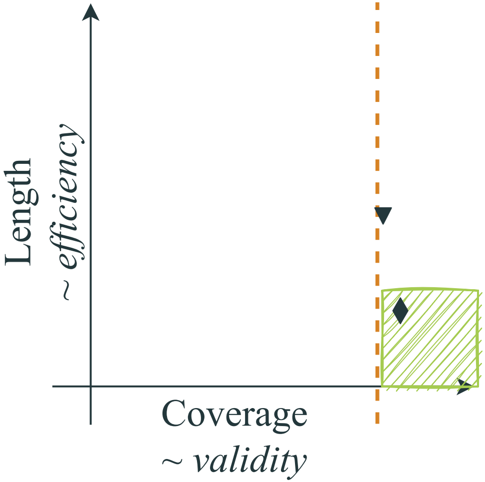

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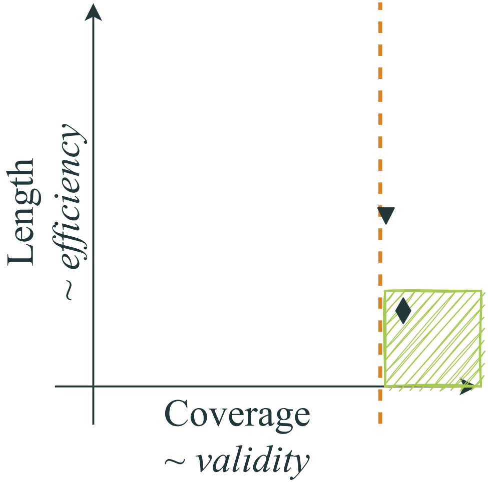

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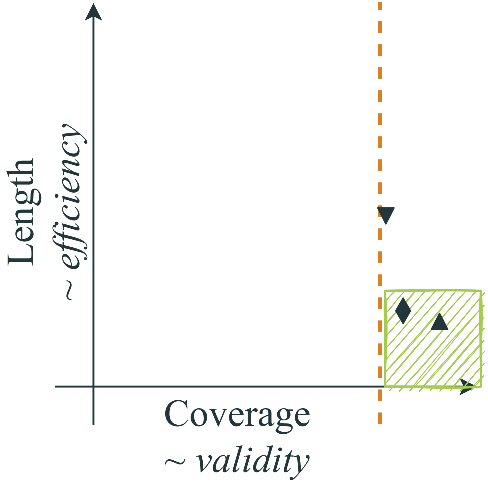

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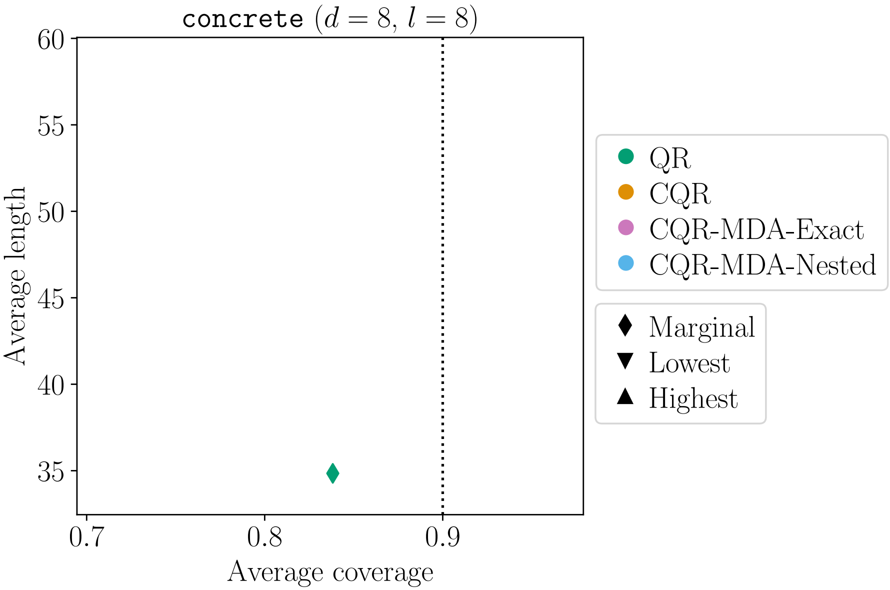
Semi-synthetic experiments



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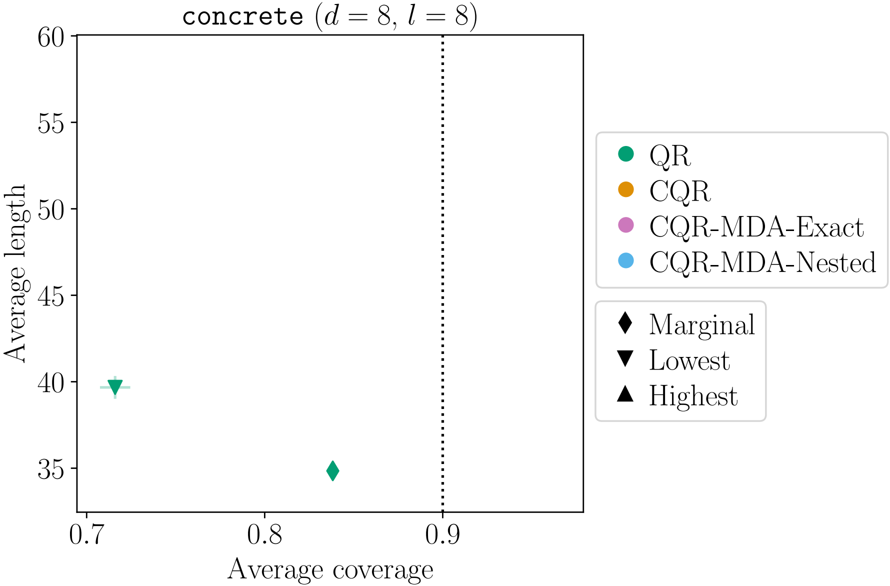

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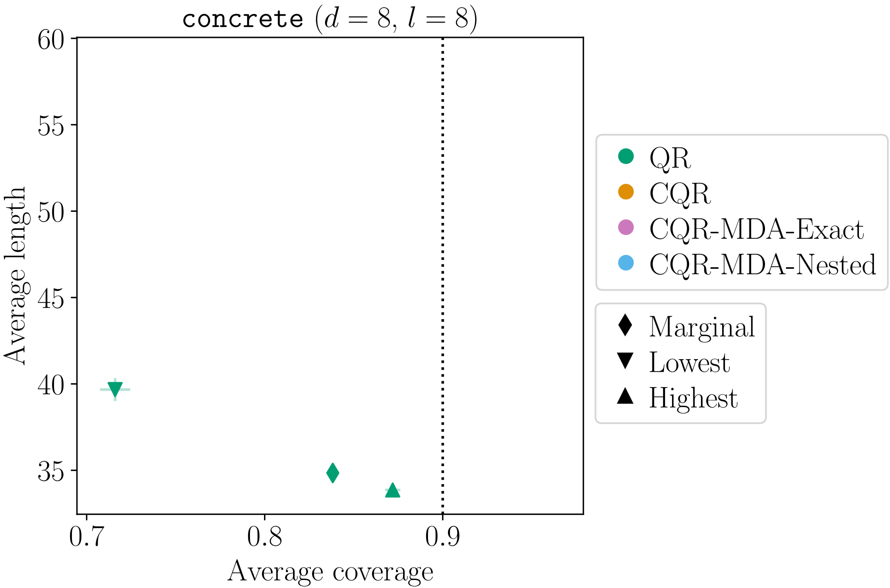

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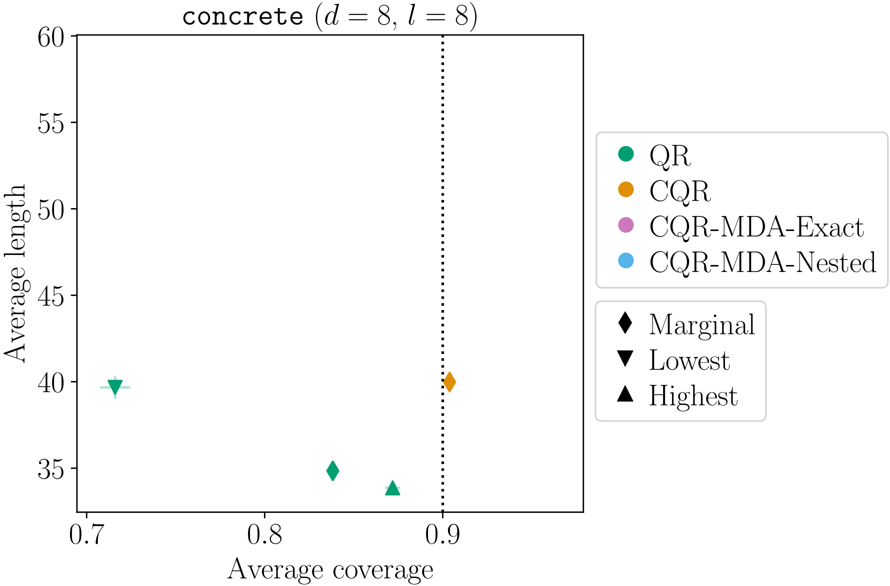

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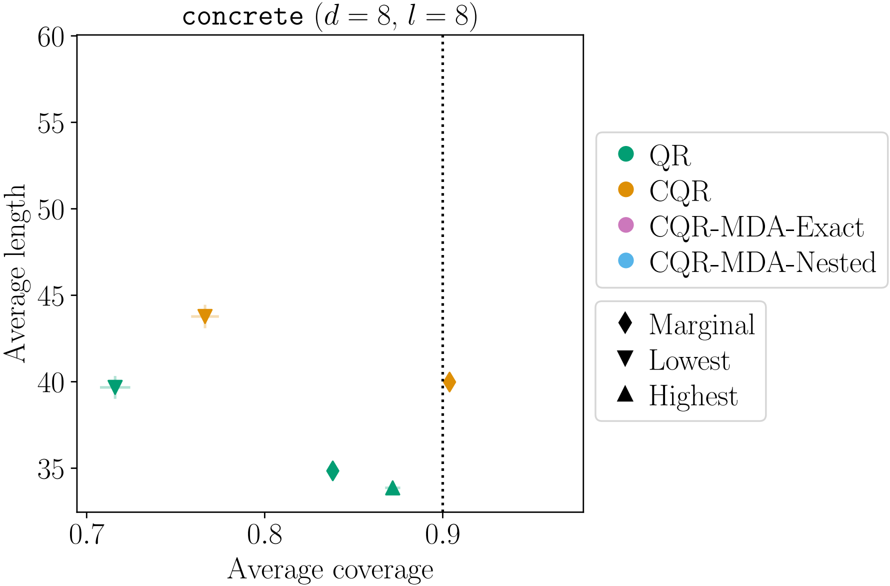

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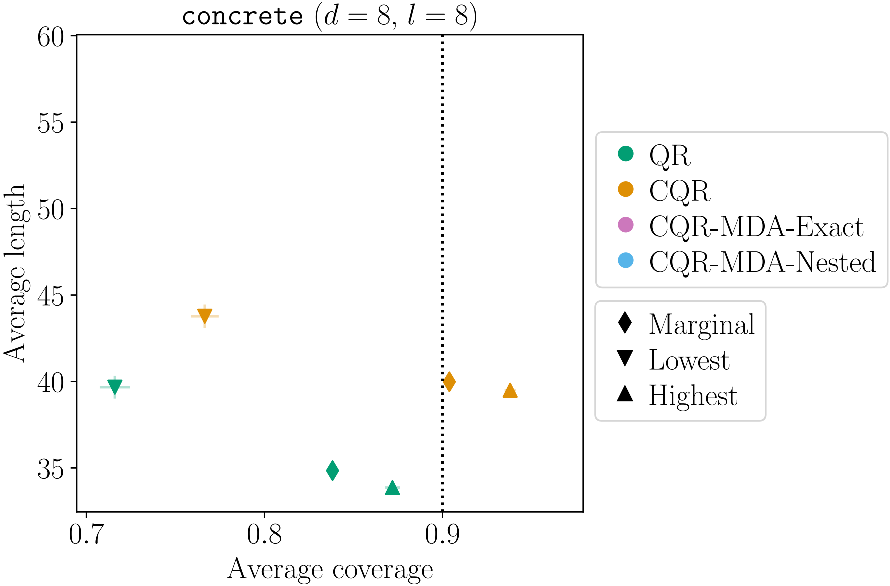

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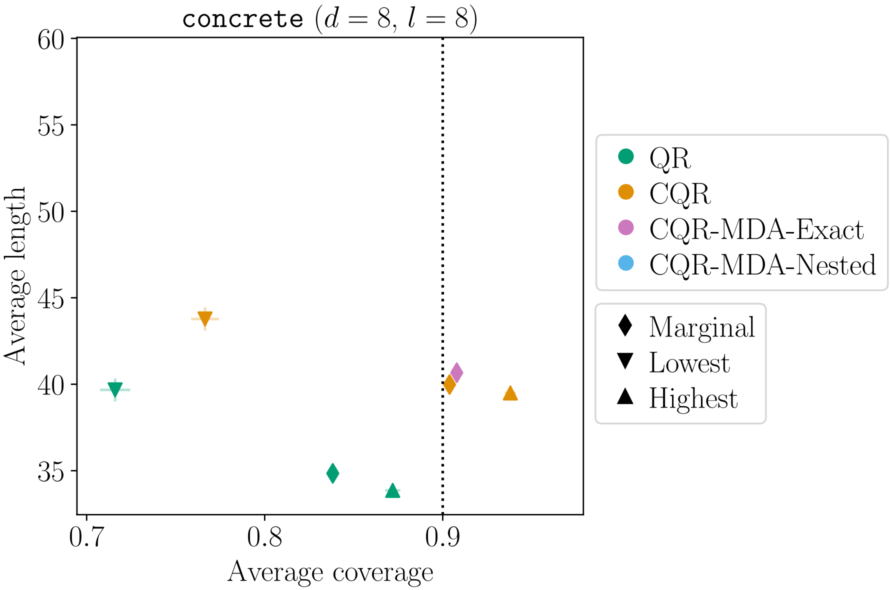
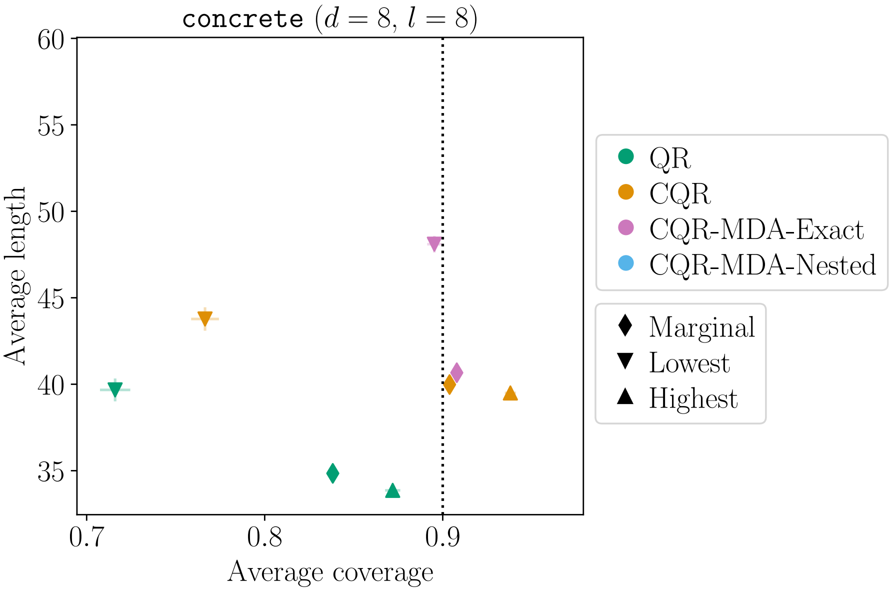
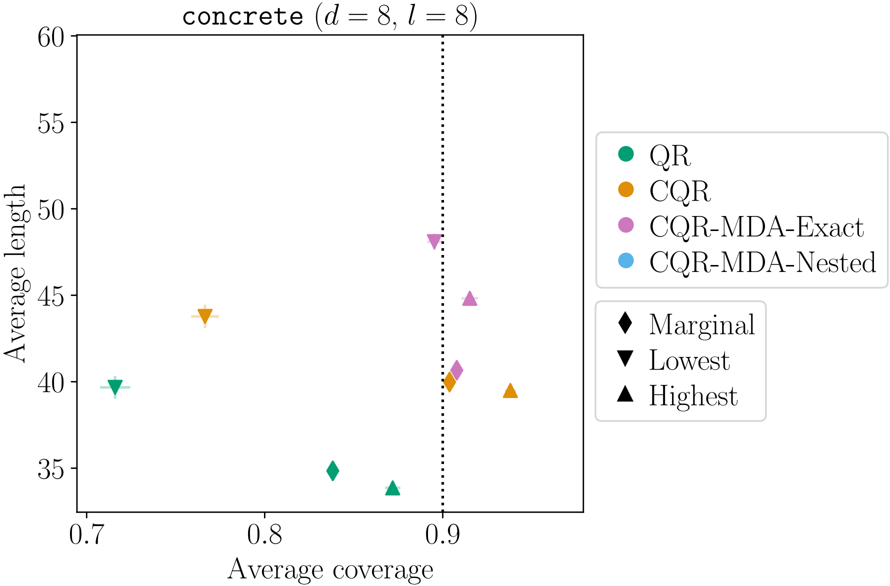




concrete ($d = 8$, $l = 8$)
60
55
50
45
40
35
Average length
0.7
0.8
0.9
Average coverage
QR
CQR
CQR-MDA-Exact
CQR-MDA-Nested
Marginal
Lowest
Highest

Semi-synthetic experiments



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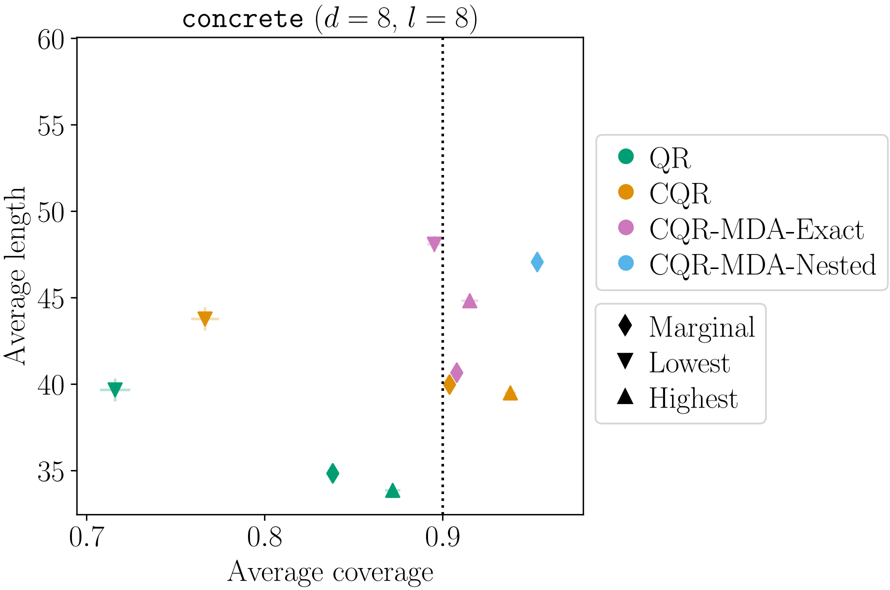

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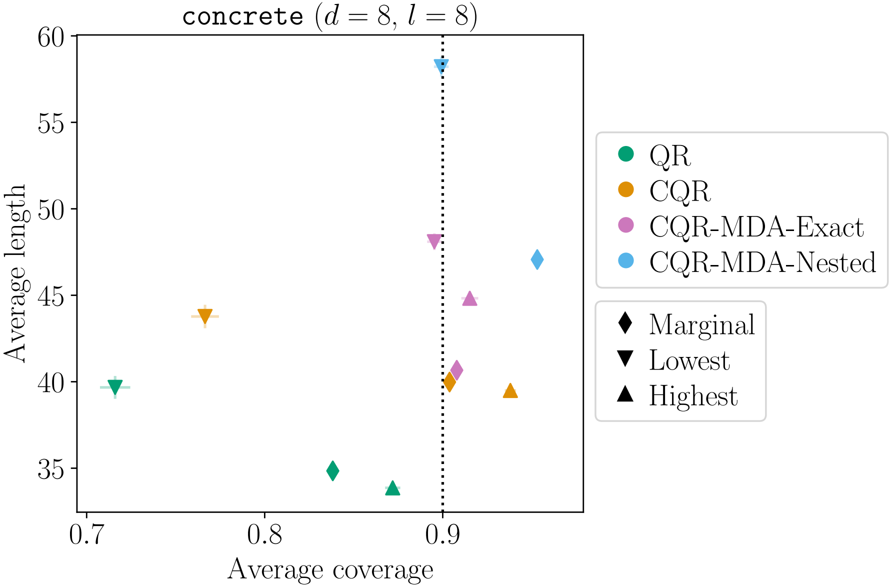

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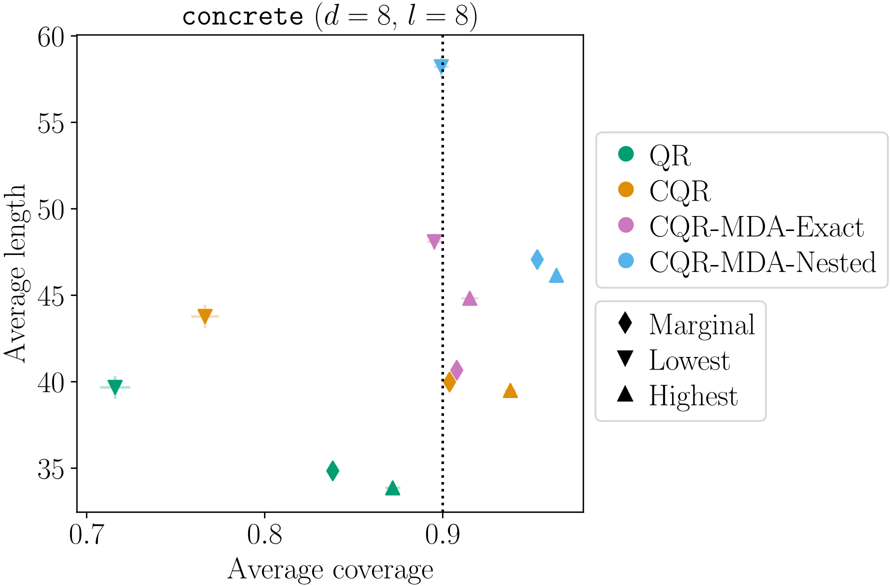
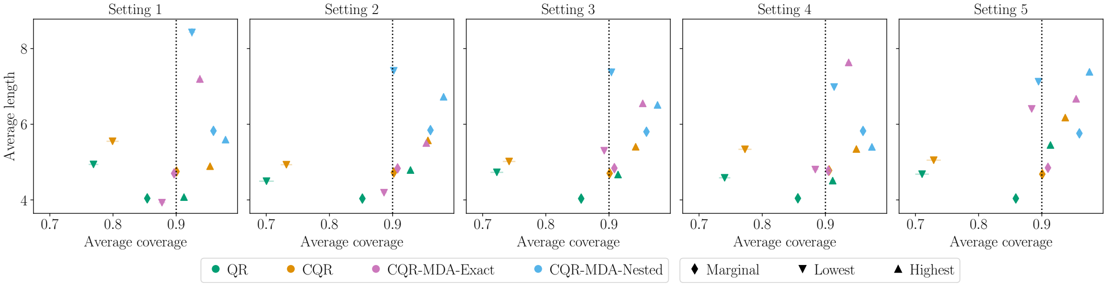


Simulation settings: beyond MCAR

- 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}.
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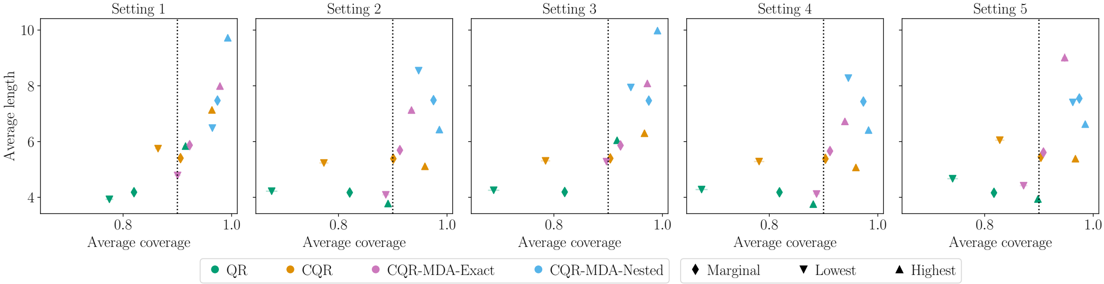
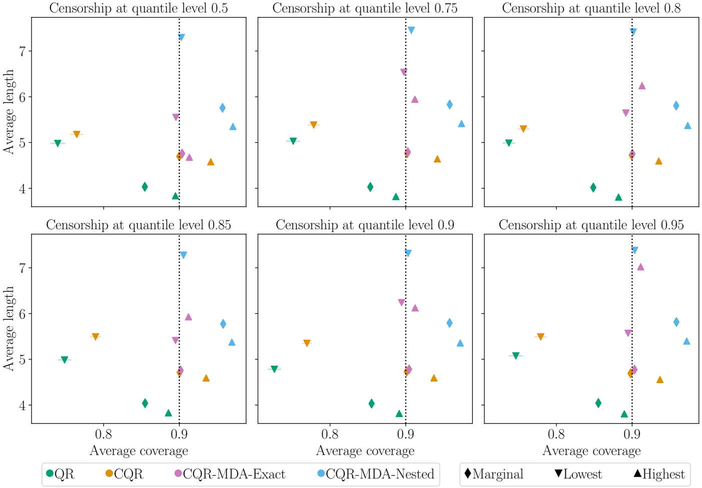


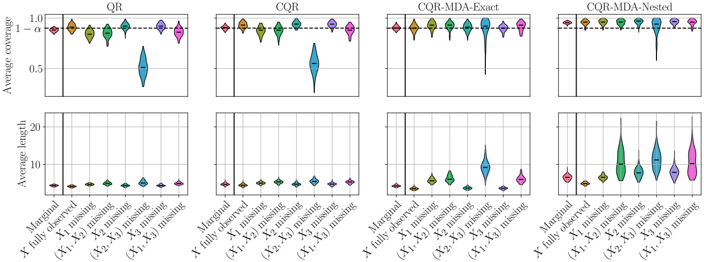
MNAR quantile censorship missingness

- 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.

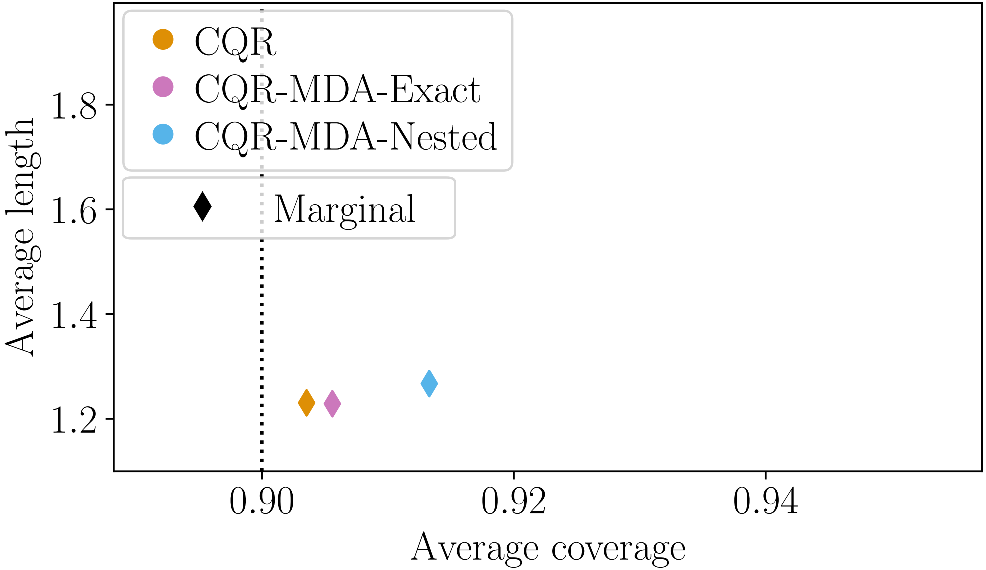


Experiments under $Y \not\perp\!\!\!\perp M \mid X$

- $M_i \sim \mathcal{B}(0.2)$ for any $i \in [\![1, 3]\!]$, independently from X and ε
- $Y = X_1 \mathbb{1}\{M_1 = 0\} + 2X_1 \mathbb{1}\{M_1 = 1\} + 3X_2 \mathbb{1}\{M_2 = 1, M_3 = 1\} + \varepsilon$



Real data experiment: TraumaBase®, critical care medicine



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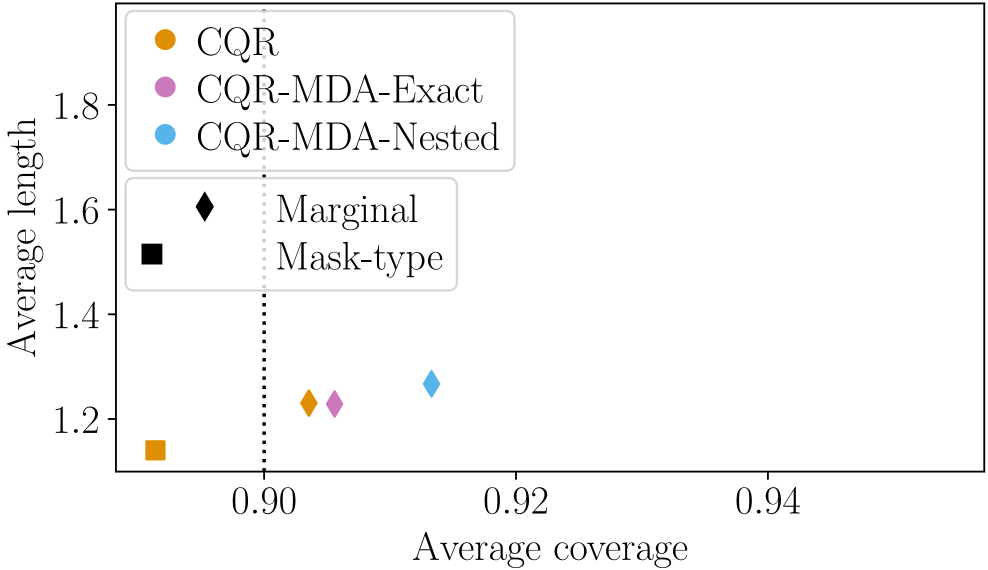

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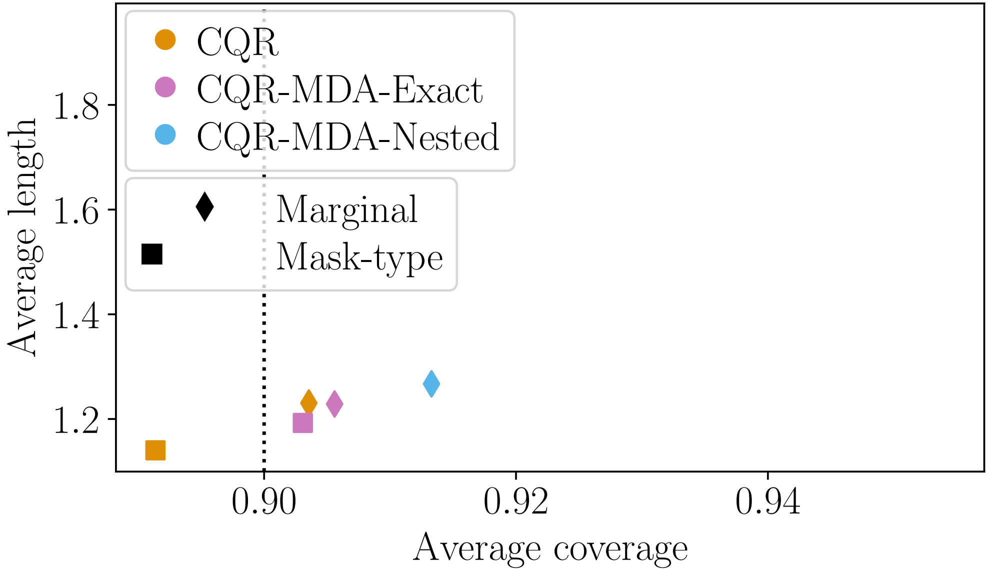

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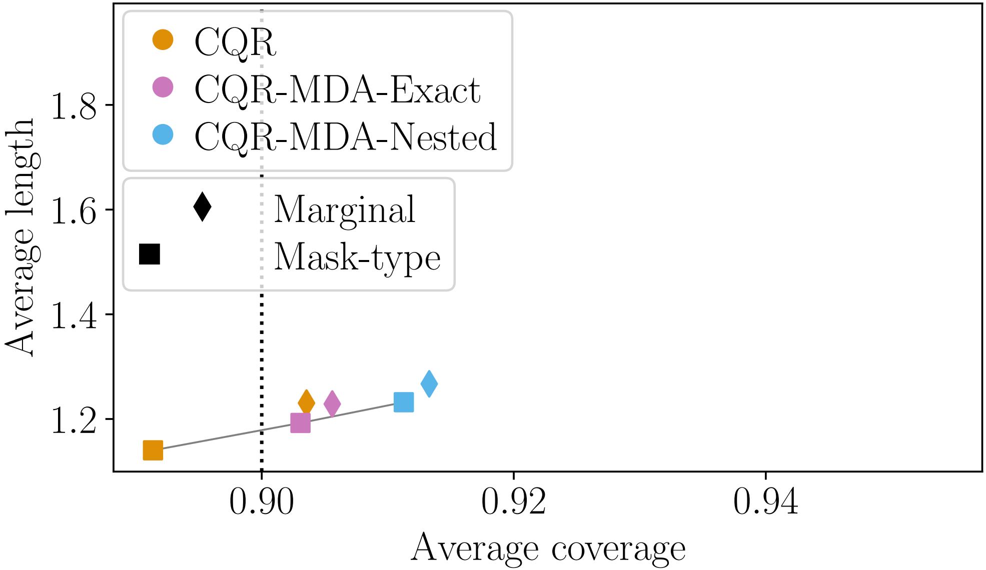
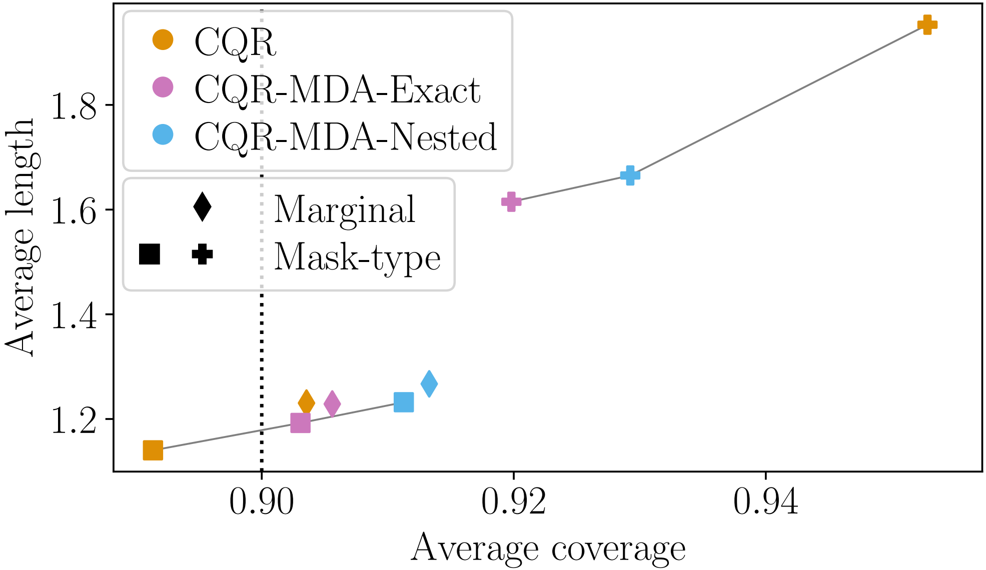
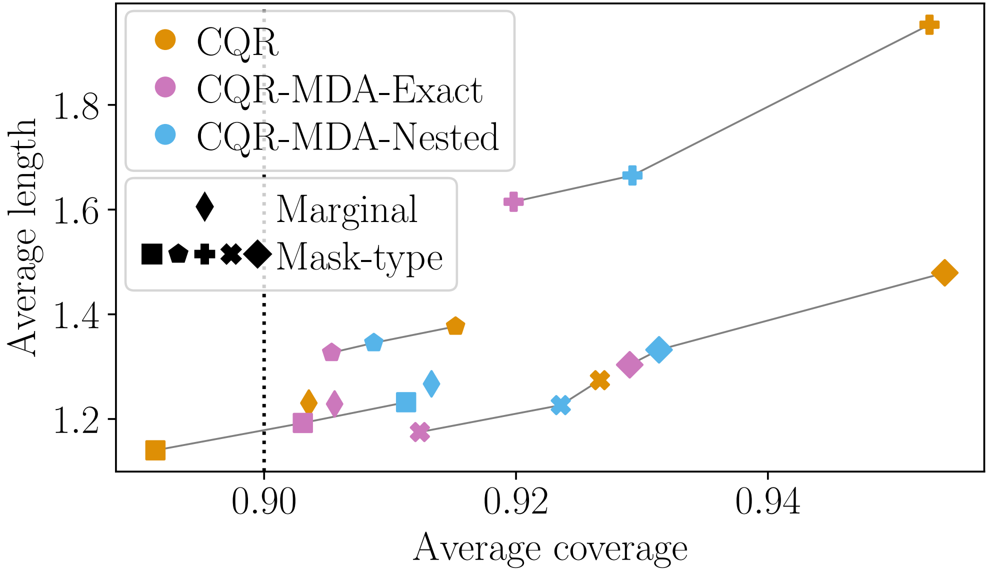


Real data experiment: TraumaBase®, critical care medicine




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

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