Simultaneous Conformal Prediction of Missing Outcomes with Propensity Score ε-Discretization

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Collaborators

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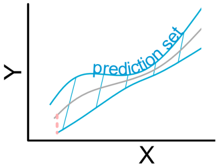

Figure: Towards DS

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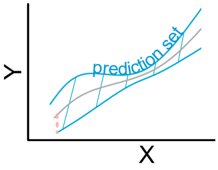

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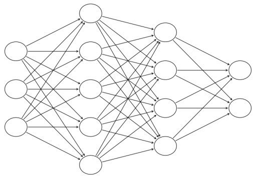

- Motivated by complex applications, e.g., where a machine learning model $\hat{\mu}$ is used to predict Y_{n+1} based on X_{n+1} (not known how to find distribution of $Y_{n+1} - \hat{\mu}(X_{n+1})$)

Introduction: Conformal prediction

- It is known how to achieve this in many settings, due to extensive work by many, starting in the 90s (Vovk, Wasserman, J. Lei, R. J. Tibshirani, Barber, Candes, ...)
- Ideas date back to work on tolerance regions by Wilks, Wald, Tukey ... starting in the 1940s


Samuel S. Wilks


Abraham Wald


Vladimir Vovk

Conformal prediction ctd.

- Typical setting: *exchangeable datapoints.*
  - For a given nonconformity score $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, e.g., $s(x, y) := |y - \hat{\mu}(x)|$, $s(X_1, Y_1), \ldots, s(X_{n+1}, Y_{n+1})$ are exchangeable (if $\hat{\mu}$ is pre-trained on an indep. dataset—i.e., in split conformal prediction)

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  - So $x \mapsto C(x) = \{y : \mathrm{rank}\{s(x, y) : s_1, \ldots, s_n\} \leq \lceil (1-\alpha)(n+1) \rceil\}$ satisfies $\mathbb{P}\{Y_{n+1} \in C(X_{n+1})\} \geq 1 - \alpha$

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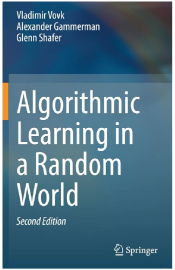

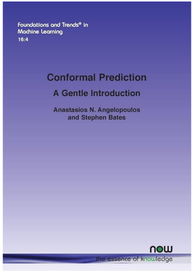

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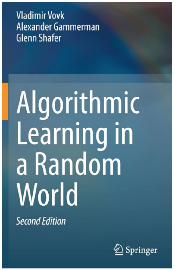
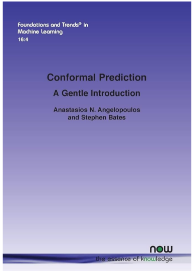
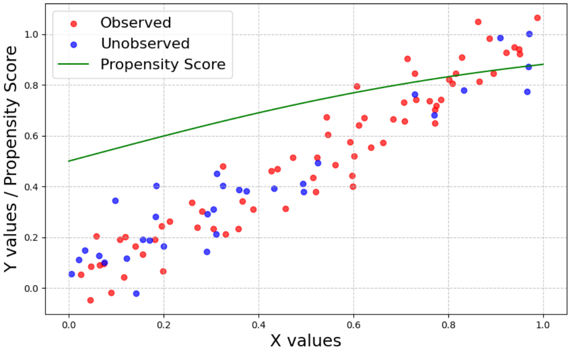




- However, there are scenarios that existing methods do not resolve, e.g., missing data

Our problem setting

- Given data
$$(X_1, A_1, Y_1A_1), \ldots, (X_n, A_n, Y_nA_n) \overset{\text{iid}}{\sim} P_X \times P_{A|X} \times P_{Y|X},$$
with outcomes *missing at random* (MAR). Thus,
$$A_i = 1 : Y_i \text{ is observed}, \qquad A_i = 0 : Y_i \text{ is unobserved}.$$



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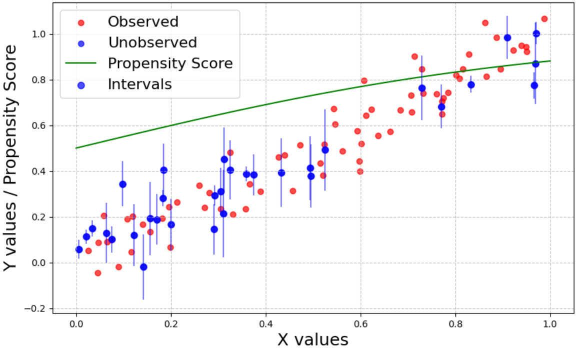
- Specifically, construct prediction sets $\{\widehat{C}(X_i) : A_i = 0\}$ for $\{Y_i : A_i = 0\}$ with coverage guarantees



Inferential target

- With i.i.d./exchangeable data $(X_1, Y_1), \cdots, (X_n, Y_n)$ and test input X_{n+1}, standard conformal prediction gives a prediction set $\widehat{C}_n(X_{n+1})$ with *marginal coverage*

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- **Question:** Under MAR:
  - In what sense can we do useful distribution-free inference for multiple unobserved outcomes?
  - Is it possible to go beyond marginal coverage? E.g., have coverage conditional on the test inputs/feature observations with missing outcomes?

Overview of results

- We consider coverage guarantees of the form

$$\mathbb{E}\left[\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i\in\widehat{C}(X_i)\right\}\,\middle|\,X_{1:n},A_{1:n}\right]\geq 1-\alpha, \tag{1}$$

  where $N^{(0)}$ is the number of unobserved labels, and $0/0 := 1$.
- The proportion of covered missing outcomes is on average at least $1-\alpha$, conditional on $X_{1:n}$ and the missingness pattern $A_{1:n}$.

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  - For discrete features X, we construct a procedure that achieves (1).
  - For general features X, we prove an impossibility result for (1); and then relax it.

Overview of results - continued

- As a relaxation, we consider

$$\mathbb{E}\left[\frac{1}{N^{(0)}} \sum_{i:A_i=0} \mathbb{1}\left\{Y_i \in \widehat{C}(X_i)\right\} \,\middle|\, B_{1:n}, A_{1:n}\right] \geq 1-\alpha, \tag{2}$$

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- **Challenge:** Even though we have MAR ($Y \perp\!\!\!\perp A \mid X$), this does not need to be preserved after discretization (may have $Y \not\perp\!\!\!\perp A \mid B$ for $B = B(X)$).
- We introduce a carefully designed propensity score partitioning scheme, and show how it can be used to obtain (2) in a distribution-free sense (for any dist. of (X, Y)).

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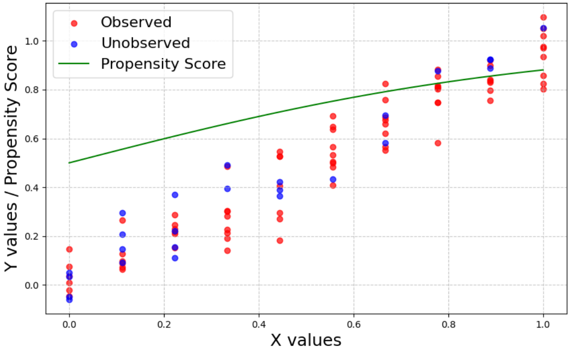
First case: Discrete features

- Discrete features naturally form groups of outcomes $\{Y_i : X_i = x\}$, $x \in \mathcal{X}$.



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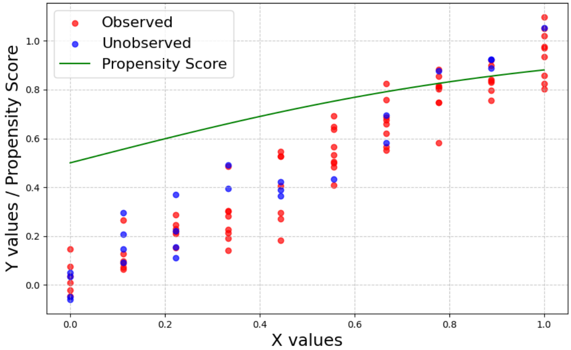
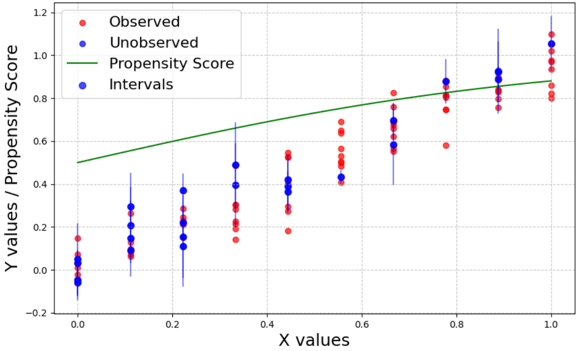


- Within each group, the outcomes are *exchangeable* conditional on $X_i = x$.

Procedure for discrete features: Naive approach

- Direct method: run split conformal prediction separately for each x.



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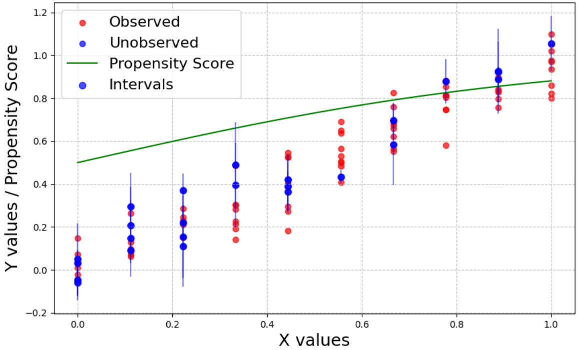

- This method attains $\mathbb{E}\left[\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i \in \widehat{C}(X_i)\right\}\,\middle|\, X_{1:n}, A_{1:n}\right] \geq 1-\alpha$.

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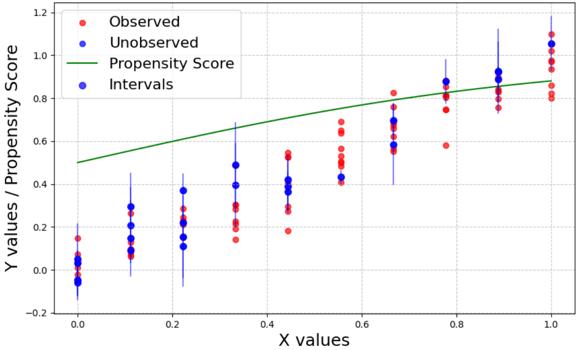

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- However, it can produce infinite-width prediction sets in small groups with $\geq \alpha$ missingness.

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  1. Nonconformity score $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, and $S_i = s(X_i, Y_i)$ if $A_i = 1$
  2. Distinct X values observed: $X'_1, \cdots, X'_M$
  3. Indices of datapoints with features equal to X'_k: $I_k = \{i \in [n] : X_i = X'_k\}$,
  4. Indices partitioned according to unobserved and observed outcomes, resp.: $I_k^0 = \{i \in [n] : X_i = X'_k, A_i = 0\}$, $I_k^1 = \{i \in [n] : X_i = X'_k, A_i = 1\}$.
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- Our prediction set:

$$\widehat{C}(x) = \left\{ y \in \mathcal{Y} : s(x, y) \le Q_{1-\alpha}\left(\sum_{k=1}^{M} \sum_{i \in I_k^1} \frac{N_k^0}{N_k N^{(0)}} \delta_{S_i} + \sum_{k=1}^{M} \frac{(N_k^0)^2}{N_k N^{(0)}} \delta_{+\infty} \right) \right\}. \quad (3)$$

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- Idea: symmetry of data distribution; see also *SymmPI* (D. & Yu, 2023)
- Provides uniform-width prediction sets for all x values.

Procedure for discrete features: guarantee

Theorem 1

The prediction set (3) satisfies *feature- and missingness-conditional coverage*

$$\mathbb{E}\left[\frac{1}{N^{(0)}} \sum_{i:A_i=0} \mathbb{1}\left\{Y_i \in \widehat{C}(X_i)\right\} \,\middle|\, X_{1:n}, A_{1:n}\right] \geq 1-\alpha.$$

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- Since guarantee is feature- and missingness-conditional, this is still valid!
- Previous methods are at two endpoints: partition is all singletons ("naive method") vs whole set ("our method").
- Why practically useful? Partition can depend on $X_{1:n}, A_{1:n}$; can aim to ensure small missingness per group.

Procedure for general feature distributions

- If the propensity score $x \mapsto p_{A|X}(x) = \mathbb{P}\{A = 1 \mid X = x\}$ is known, ε-**discretize** it
- Let ε be a predefined discretization level, and $z_k = (1+\varepsilon)^k/[1+(1+\varepsilon)^k]$ for all integers k

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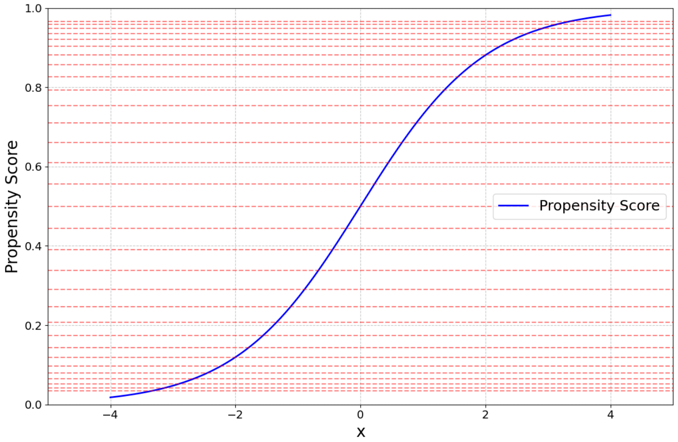

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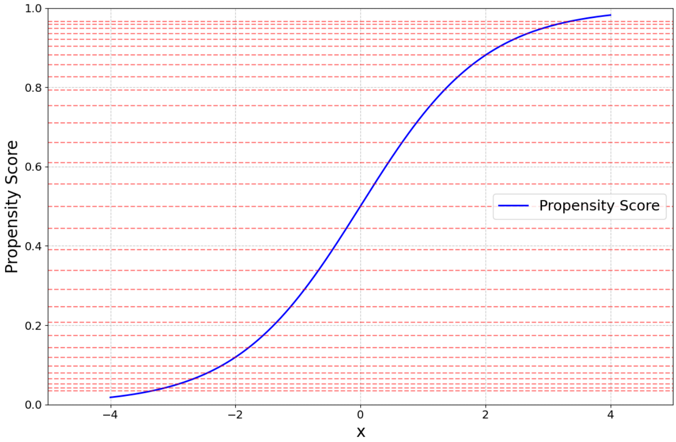

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Theorem 2

Suppose $0 < p_{A|X}(X) < 1$ almost surely. Then $\widehat{C}^{\text{pro-CP}}$ from (4) satisfies *propensity score discretized feature- and missingness-conditional coverage*:

$$\mathbb{E}\left[\frac{1}{N^{(0)}} \sum_{i:A_i=0} \mathbb{1}\left\{ Y_i \in \widehat{C}^{\text{pro-CP}}(X_i) \right\} \,\middle|\, B_{1:n}, A_{1:n} \right] \ge 1 - \alpha - \varepsilon.$$

Pro-CP

- Show *approximate within-partition exchangeability* of the scores, enabling inference.
- **Propensity score discretization-based conformal prediction (pro-CP)**: Procedure (4) applied to the discretized data $(B_i, A_i, A_i Y_i)_{i \in [n]}$, i.e.,

$$\widehat{C}^{\text{pro-CP}}(x) = \left\{ y \in \mathcal{Y}, :, s(x,y) \leq Q_{1-\alpha}\left(\sum_{k=1}^{M} \sum_{i \in I_k^{\mathcal{B},1}} \frac{N_k^{\mathcal{B},0}}{N^{(0)} N_k^{\mathcal{B}}} \cdot \delta_{S_i} + \frac{1}{N^{(0)}} \sum_{k=1}^{M} \frac{(N_k^{\mathcal{B},0})^2}{N_k^{\mathcal{B}}} \cdot \delta_{+\infty} \right) \right\}. \tag{4}$$

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- The error from discretization is bounded by ε, for *any* n and $\#$ of missing outcomes.

Pro-CP with estimated propensity score

- If the propensity score is unknown, we may run pro-CP with an estimator $\hat{p}_{A|X}$ of $p_{A|X}$.

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where

$$\delta_{\hat{p}_{A|X}} = e^{2\|\log f_{p,\hat{p}}\|_\infty} - 1, \qquad f_{p,\hat{p}}(x) = \frac{p_{A|X}(x)/(1-p_{A|X}(x))}{\hat{p}_{A|X}(x)/(1-\hat{p}_{A|X}(x))}.$$

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- The error from estimation does not grow with the number of missing outcomes.

New result underlying pro-CP guarantee

- Balancing property of the propensity score [Rosenbaum and Rubin (1983)]: the missingness is independent of the outcome conditional on the propensity: $A \perp\!\!\!\perp Y \mid p_{A|X}$.

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- Balancing property of the propensity score [Rosenbaum and Rubin (1983)]: the missingness is independent of the outcome conditional on the propensity: $A \perp\!\!\!\perp Y \mid p_{A|X}$.
- We show *approximate version*: dist. of $s(X, Y)$ close for $A = 0, 1$ given small range of $p_{A|X}$

Lemma (Bounded prop. score implies closeness of cond. distrib. for obs. and missing)

Suppose that $(X, Y, A) \sim P_X \times P_{Y|X} \times \text{Bernoulli}(p_{A|X})$ *on* $\mathcal{X} \times \mathcal{Y} \times \{0, 1\}$, *and that for a set* $B \subset \mathcal{X}$ *and* $t \in (0, 1)$, $\varepsilon \geq 0$,

$$t \leq \frac{p_{A|X}(x)}{1 - p_{A|X}(x)} \leq t(1 + \varepsilon), \text{ for all } x \in B.$$

Let $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ *be any measurable function and let* $S = s(X, Y)$. *Then*

$$d_{TV}(P_{S|A=1,X\in B}, P_{S|A=0,X\in B}) \leq \varepsilon.$$

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Application to simultaneous inference on ITEs

- Consider a potential outcomes model

$$(X_i, T_i, Y_i(0), Y_i(1))_{1 \le i \le n} \overset{\text{iid}}{\sim} P_X \times P_{T|X} \times P_{Y(1)|X} \times P_{Y(0)|X},$$

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- Applying pro-CP, we can construct $\widehat{C}^{\text{counterfactual}}$ such that

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- By letting $\widehat{C}_i^{\text{ITE}} = \{y - Y_i(0) : y \in \widehat{C}^{\text{counterfactual}}(X_i)\}$, we obtain prediction sets for individual treatment effects

$$\mathbb{E}\left[\tfrac{1}{N^{(0)}} \textstyle\sum_{i\in I_{T=0}} \mathbb{1}\left\{(Y_i(1) - Y_i(0)) \in \widehat{C}_i^{\text{ITE}}\right\} \,\middle|\, B_{1:n}, T_{1:n}\right] \geq 1 - \alpha.$$

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$$\mathbb{P}\left\{\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i\in\widehat{C}^{\text{pro-CP}}(X_i)\right\}\geq 1-\alpha\right\}\geq 1-\delta.$$

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(motivated by Lee et. al. (2023): Hierarchical CP)

Interpretation of the squared-coverage guarantee

- Let $\hat{m} = \frac{1}{N^{(0)}} \sum_{i:A_i=0} \mathbb{1}\left\{Y_i \in \widehat{C}^{\text{pro-CP}}(X_i)\right\}$ denote the *miscoverage proportion*.

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- Conditional on (discretized) features, pro-CP attains $\mathbb{E}[\hat{m}] \leq \alpha$.
- The squared-coverage guarantee is $\mathbb{E}\left[\hat{m}^2\right] \leq \alpha^2$, and provides a stronger control over $\hat{m}$ being close to unity, preventing e.g., $\hat{m} = 0$ w.p. $1 - \alpha$ and 1 w.p. α.

Pro-CP2 procedure

- Define
  1. For all $i \in [n]$, $\bar{S}_i = S_i$ if $A_i = 1$ and $\bar{S}_i = +\infty$ if $A_i = 0$.
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- Pro-CP2 prediction set:

$$\widehat{C}^{\text{pro-CP2}}(x) = \Bigg\{ y \in \mathcal{Y} : s(x,y) \le Q_{1-\alpha^2} \Bigg(\sum_{k=1}^{M} \sum_{i \in I_k^{\mathcal{B}}} \frac{1}{(N^{(0)})^2} \cdot \frac{N_k^{\mathcal{B},0}}{N_k^{\mathcal{B}}} \cdot \delta_{\bar{S}_i}$$

$$+ \sum_{k=1}^{M} \sum_{\substack{i,j \in I_k^{\mathcal{B}} \\ i \neq j}} \frac{N_k^{\mathcal{B},0}(N_k^{\mathcal{B},0} - 1)}{(N^{(0)})^2 N_k^{\mathcal{B}} (N_k^{\mathcal{B}} - 1)} \delta_{\bar{S}_{ij}} + \sum_{1 \le k \neq k' \le M} \sum_{i \in I_k^{\mathcal{B}}} \sum_{j \in I_{k'}^{\mathcal{B}}} \frac{N_k^{\mathcal{B},0} N_{k'}^{\mathcal{B},0}}{(N^{(0)})^2 N_k^{\mathcal{B}} N_{k'}^{\mathcal{B}}} \delta_{\bar{S}_{ij}} \Bigg) \Bigg\}.$$

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$$\left.\left. + \sum_{k=1}^{M} \sum_{\substack{i,j \in I_k^{\mathcal{B}} \\ i \neq j}} \frac{N_k^{\mathcal{B},0}(N_k^{\mathcal{B},0} - 1)}{(N^{(0)})^2 N_k^{\mathcal{B}}(N_k^{\mathcal{B}} - 1)} \delta_{\bar{S}_{ij}} + \sum_{1 \leq k \neq k' \leq M} \sum_{i \in I_k^{\mathcal{B}}} \sum_{j \in I_{k'}^{\mathcal{B}}} \frac{N_k^{\mathcal{B},0} N_{k'}^{\mathcal{B},0}}{(N^{(0)})^2 N_k^{\mathcal{B}} N_{k'}^{\mathcal{B}}} \delta_{\bar{S}_{ij}} \right) \right\}.$$

- Similar intuition as before; but use invariance to find probability of $\mathbb{1}\left\{\min\{S_{i^*}, S_{j^*}\} \leq q_{1-\alpha^2}(\tilde{S}_1, \ldots, \tilde{S}_M)\right\}$, where i^*, j^* are random data indices with $A = 0$.

Squared coverage error control of Pro-CP2

Theorem 4

If $0 < p_{A|X}(X) < 1$ almost surely, then $\widehat{C}^{\text{pro-CP2}}$ satisfies

$$\mathbb{E}\left[\left(\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i \notin \widehat{C}^{\text{pro-CP2}}(X_i)\right\}\right)^2 \,\middle|\, B_{1:n}, A_{1:n}\right] \le \alpha^2 + 2\varepsilon.$$

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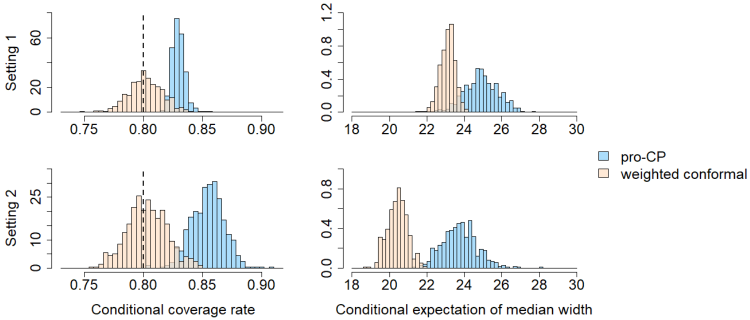


Simulation 2

pro-CP vs pro-CP2: controlling mean vs squared miscoverage

- Same setting as Simulation 1, but evaluate marginal coverage & estimate propensity score with kernel regression on training data

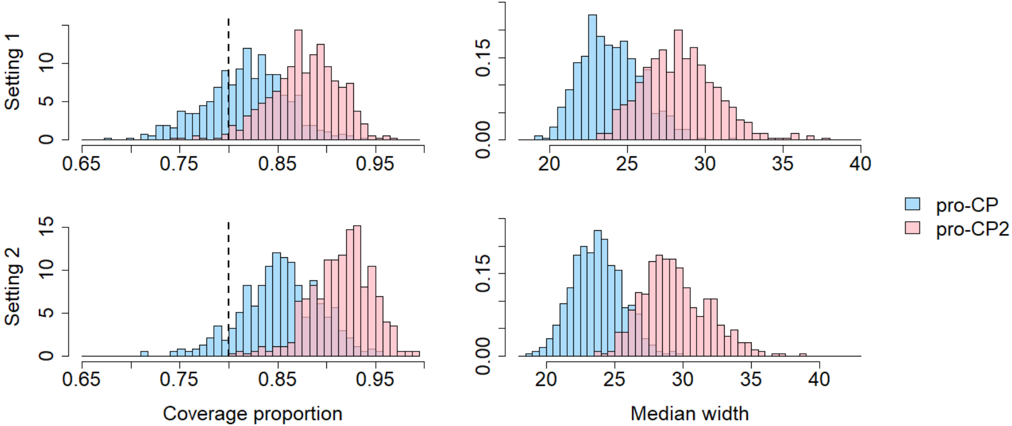


Illustration on diabetes dataset (Efron et al., 2004)

- X: ten features (age, bmi, LDL/HDL, ...) of patients (sample sizes: train: 142; calibration+test: 300)
- A: missingness generated from a known logistic model
- Y: a measure of disease progression one year after baseline

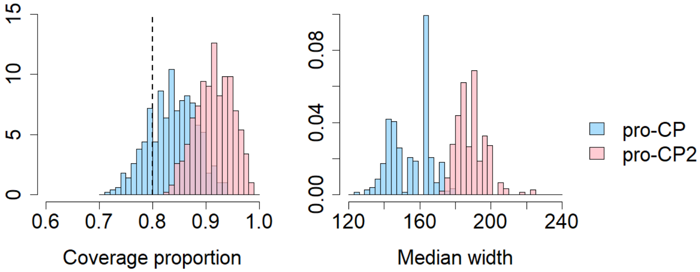


Illustration on diabetes dataset (Efron et al., 2004): II

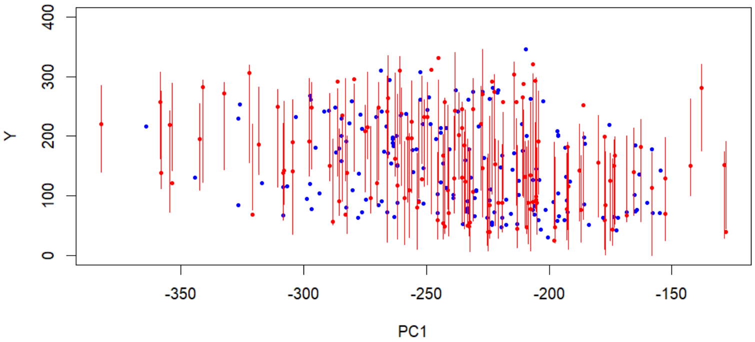
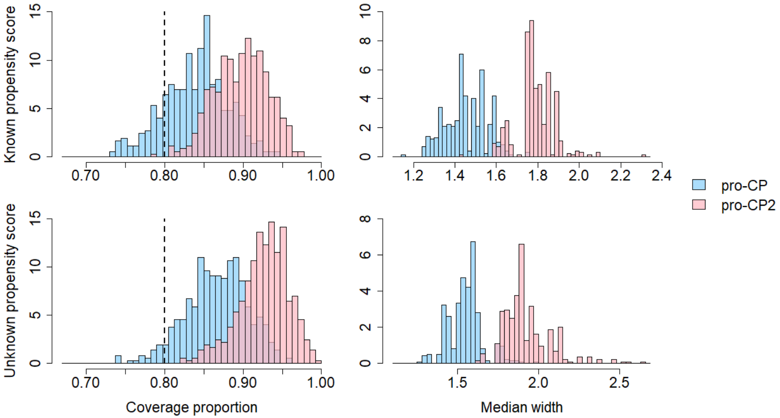


Illustration on JOBS II dataset (Imai et al., 2010)

- X: job seekers: $n_{\text{train}} = 379$, $n = 500$; with 14 demographic features
- A: job skills workshop (to evaluate our methods, simulate via logistic model; estimate via RF)
- $Y(0), Y(1)$: pre- and post-treatment depression measure



Discussion

- Introduced Pro-CP, a method for simultaneous prediction of multiple missing outcomes, and provided coverage guarantees
- Pro-CP2: stronger squared error miscoverage error control
- What applications might this have an impact on? Where could it be used?
- Preprint: `arxiv.org/abs/2403.04613`. Code: `github.com/yhoon31/pro-CP`
- Thanks!

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