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

Edgar Dobriban

Department of Statistics and Data Science, the Wharton School, University of Pennsylvania

July 19, 2024

Collaborators

Yonghoon Lee

Eric Tchetgen Tchetgen

Table of Contents

Introduction and Overview

Our Methods

Illustrating Our Methods in a Stylized Problem

A Stronger Guarantee

Empirical illustration

Introduction: Conformal prediction

- Major developing area in statistics: distribution-free predictive inference (a.k.a. conformal prediction)
- Goal, given $(X_1, Y_1), \ldots, (X_n, Y_n)$, find a prediction set C such that for new X_{n+1}, $\mathbb{P}\{Y_{n+1} \in C(X_{n+1})\} \geq 1 - \alpha$ under *minimal assumptions*

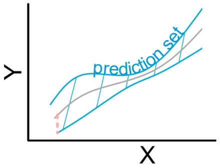
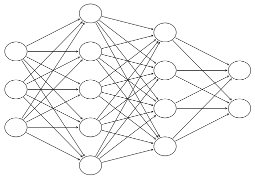


Figure: Towards DS



- 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—a.k.a. split conformal prediction)
  - Hence, the rank of $s(X_{n+1}, Y_{n+1})$ is uniform over $1, \ldots, n+1$ (if no ties)
  - So $x \mapsto C(x) = \{y : \mathrm{rank}\{s(x, y) : s_1, \ldots, s_n\} \leq \lceil (1-\alpha)(n+1) \rceil\}$ satisfies $\mathbb{P}\{Y_{n+1} \in C(X_{n+1})\} \geq 1 - \alpha$
- See e.g., tutorial by Angelopoulos & Bates
- However, there are many important scenarios that existing methods do not fully address, e.g., missing data

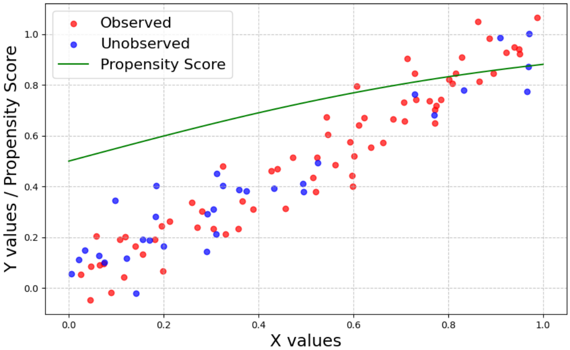
Our problem setting

- Given data

$$(X_1, A_1, Y_1A_1), \ldots, (X_n, A_n, Y_nA_n) \overset{\text{iid}}{\sim} P_X \times P_{A|X} \times P_{Y|X},$$

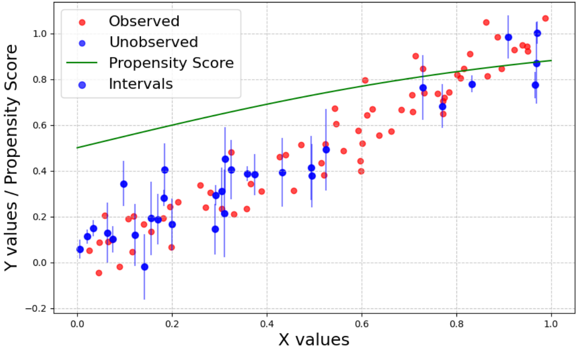
with outcomes *missing at random* (MAR). Thus,

$$A_i = 1 : Y_i \text{ is observed}, \qquad A_i = 0 : Y_i \text{ is unobserved}.$$



Our problem setting

- **Goal**: Simultaneous inference on the missing outcomes $\{Y_i : A_i = 0\}$.
- Specifically, construct prediction sets $\{\widehat{C}(X_i) : A_i = 0\}$ for $\{Y_i : A_i = 0\}$ with a useful guarantee



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*

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

- **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 $A_{1:n}$.
  - 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

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

  where B_i is a discretization of X_i (defined soon).

- **Challenge:** Even though we have MAR ($Y \perp\!\!\!\perp A \mid X$), this does not need to be preserved after discretization (may have $Y \not\perp\!\!\!\perp A \mid B$).
- 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)).

Table of Contents

Introduction and Overview

Our Methods

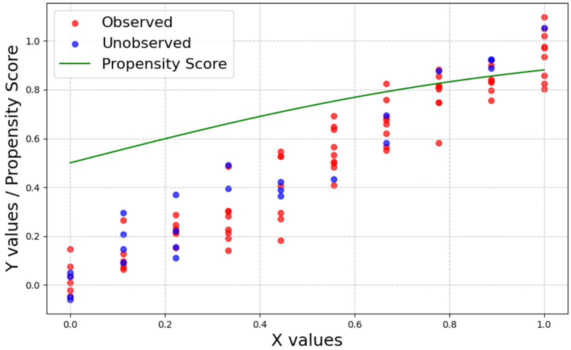
Illustrating Our Methods in a Stylized Problem

A Stronger Guarantee

Empirical illustration

Discrete features

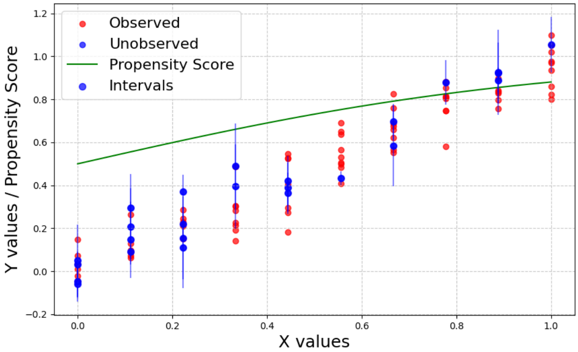
- Discrete features naturally form groups of outcomes $\{Y_i : X_i = x\}$, $x \in \mathcal{X}$.



- 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.



- This method attains $\mathbb{E}\left[\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i \in \widehat{C}(X_i)\right\} \,\middle|\, X_{1:n}, A_{1:n}\right] \geq 1-\alpha$.
- However, it can produce infinite-width prediction sets for outcomes in small groups.

Procedure for discrete features: our method

- Alternative method: simultaneous inference across multiple feature values.
- Let
  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.: $I_k^0 = \{i \in [n] : X_i = X'_k, A_i = 0\}$, $I_k^1 = \{i \in [n] : X_i = X'_k, A_i = 1\}$.
  5. Their sizes $N_k = |I_k|$, $N_k^0 = |I_k^0|$,
- Our prediction set:

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

- 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*

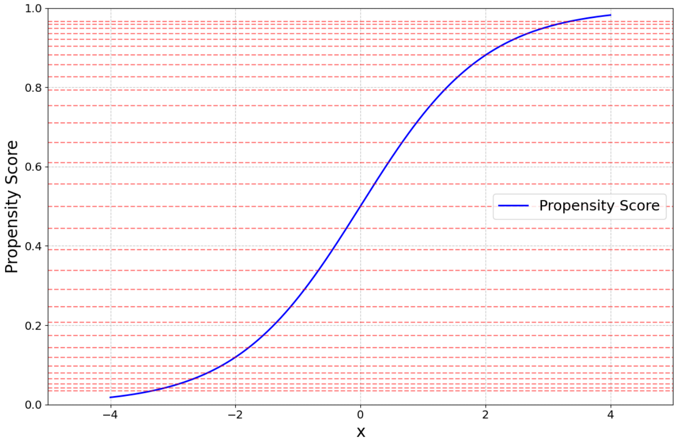
$$\mathbb{E}\left[\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i\in\widehat{C}(X_i)\right\}\,\middle|\,X_{1:n},A_{1:n}\right]\geq 1-\alpha.$$

Discrete features: improvement via partitioning

- If missingness proportion is high, this can still be conservative.
- Idea: *Partition* datapoints. For each partition, use pro-CP on *all datapoints with observed labels* to predict outcomes missing in that partition.
- Since guarantee is feature- and missingness-conditional, this is valid!
- Previous methods are at two endpoints: partition is all singletons ("naive method") vs whole set ("our method").
- 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
- Partition the feature space into $D_k = \left\{x : p_{A|X}(x) \in [z_k, z_{k+1})\right\}$, $\mathcal{B} = \{D_k : k \in \mathbb{Z}\}$.



Pro-CP

- Have *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.,

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

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*

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

- 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 $p_{A|X}$.

Theorem 3

Suppose $0 < p_{A|X}(X) < 1$ and $0 < \hat{p}_{A|X}(X) < 1$ almost surely. Then pro-CP run with $\hat{p}_{A|X}$ satisfies

$$\mathbb{E}\left[\frac{1}{N^{(0)}} \sum_{i:A_i=0} \mathbb{1}\left\{Y_i \in \widehat{C}^{\text{pro-CP}}(X_i)\right\} \,\middle|\, B_{1:n}, A_{1:n}\right] \geq 1 - \alpha - (\varepsilon + \delta_{\hat{p}_{A|X}} + \varepsilon\delta_{\hat{p}_{A|X}}),$$

where

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

- 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: $A \perp\!\!\!\perp Y \mid p_{A|X}$.
- 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 $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ *by any measurable function and let* $S = s(X, Y)$. *Then*

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

Table of Contents

Introduction and Overview

Our Methods
- Illustrating Our Methods in a Stylized Problem
- A Stronger Guarantee

Empirical illustration

Application to simultaneous inference on ITEs

- Consider a potential outcomes model

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

  where we observe $(X_i, T_i, T_i Y_i(1) + (1 - T_i) Y_i(0))_{1\le i\le n}$.

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

$$\mathbb{E}\left[\tfrac{1}{N^{(0)}} \textstyle\sum_{i:\, T_i=0} \mathbb{1}\left\{Y_i(1) \in \widehat{C}^{\text{counterfactual}}(X_i)\right\} \;\middle|\; B_{1:n}, T_{1:n}\right] \ge 1 - \alpha.$$

- 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

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

Table of Contents

Introduction and Overview

Our Methods

Illustrating Our Methods in a Stylized Problem

A Stronger Guarantee

Empirical illustration

Achieving a stronger guarantee on the coverage proportion

- Can we achieve a stronger guarantee beyond bounding the *mean coverage*?
- Example: PAC-type guarantee of the form

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

- Turns out to be hard to achieve in the distribution-free sense
- As a surrogate target, we consider bounding the *squared coverage*

$$\mathbb{E}\left[\left(\frac{1}{N^{(0)}}\sum_{i:A_i=0}\mathbb{1}\left\{Y_i \notin \widehat{C}^{\text{pro-CP}}(X_i)\right\}\right)^2\right] \leq \alpha^2.$$

(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*.
- Conditional on (discretized) features, pro-CP attains $\mathbb{E}\left[\hat{m}\right] \le \alpha$.
- The squared-coverage guarantee is $\mathbb{E}\left[\hat{m}^2\right] \le \alpha^2$, and provides a stronger control over $\hat{m}$ being close to unity, e.g., prevents cases such as $\hat{m} = 0$ 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 $A_i = 0$.
  2. Pairwise minima: $\bar{S}_{ij} := \min\{\bar{S}_i, \bar{S}_j\}$ for all i, j.
- Pro-CP2 prediction set:

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

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

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

Table of Contents

Introduction and Overview

Our Methods

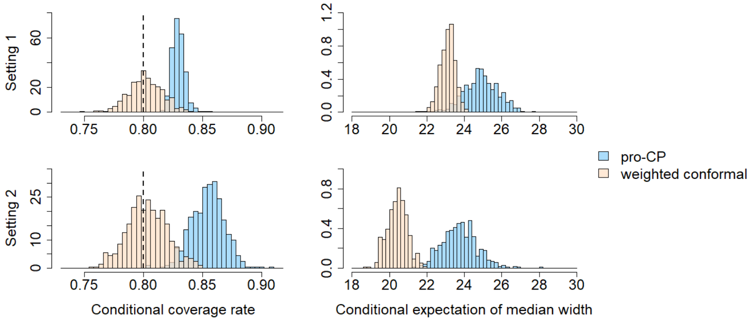
- Illustrating Our Methods in a Stylized Problem
- A Stronger Guarantee

Empirical illustration

Simulation 1

Weighted conformal (Tibshirani et al., 2019) vs pro-CP: marginal vs conditional coverage

1. $X \sim \text{Unif}[0,10]$, $Y \mid X \sim N(X,(3+X)^2)$, $A \mid X \sim \text{Bernoulli}(p_{A|X}(X))$
2. $(1): p_{A|X}(x) = 0.9 - 0.02x$, $(2): p_{A|X}(x) = 0.8 - 0.1(1+0.1x)\sin 3x$
3. Fit lin. reg. with $n_{\text{train}} = 500$, $s(x,y) = |y - \hat{\mu}(x)|$
4. 500 trials, $n = 500$, Pro-CP $\varepsilon = 0.1$, $\alpha = 0.2$, partition of size 10;
5. given $X_{1:n}, A_{1:n}$, 100x gen $(X_i', Y_i')_{1<i<n} \mid B_i \sim P_{X|B} \times P_{Y|X}$, $n = 500$



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

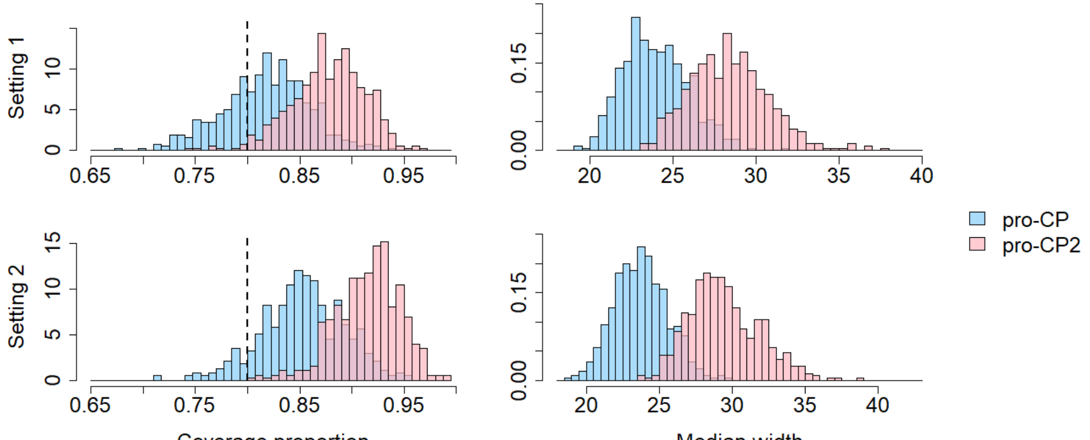


Illustration on diabetes dataset (Efron et al., 2004)

- 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

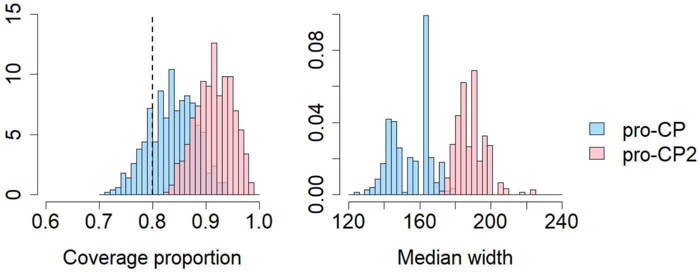
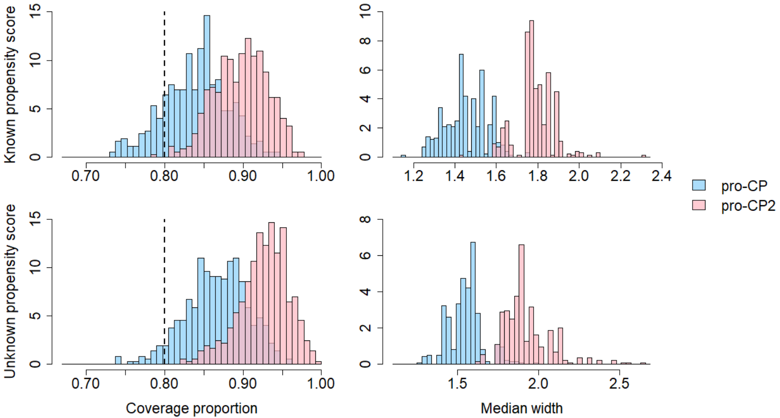


Illustration on JOBS II dataset (Imai et al., 2010)

- X: job seekers: $n_{\mathrm{train}} = 379$, $n = 500$; in 14 dimensions (demographics)
- 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
- Preprint: `arxiv.org/abs/2403.04613`. Code: `github.com/yhoon31/pro-CP`
- Thanks!