Distribution-Free Prediction Sets Adaptive to Unknown Covariate Shift

Hongxiang Qiu, Edgar Dobriban, Eric Tchetgen Tchetgen

Department of Statistics, The Wharton School, University of Pennsylvania

Motivation

- Great advances in prediction using machine learning
- Prediction sets with coverage guarantees are useful to quantify uncertainty of prediction
- One useful guarantee is *Probably Approximately Correct* (PAC):

$$\Pr\left(\Pr\left(Y \notin \hat{C}(X) \mid \text{training data}\right) \leq \alpha_{\text{error}}\right) \geq 1 - \alpha_{\text{conf}}$$

- Interpretation: with high confidence level $1 - \alpha_{\text{conf}}$ (*probably*), the coverage error rate of $\hat{C}$ is below α_{error} (*approximately correct*)
- Also termed "training-set conditional validity"
- Inductive conformal prediction outputs PAC prediction sets if all data come from the same population [Papadopoulos et al., 2002, Vovk, 2013, Park et al., 2020]

Motivation

- Challenge: in many applications, labeled training data are drawn from a different population from the target population
- For example, labeled data from Africa but want to predict in USA
- Common assumption: covariate shift (covariate distribution shifts; distribution of label/outcome given covariate remains same)
- Under covariate shift, we learn $Y \mid X$ using labeled data from source population and can extrapolate to target population

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- Previous literature: Sort of: require knowing exactly the covariate distribution shift [Park et al., 2021]
- What if this shift is unknown?
- Available data: i.i.d. from P^0
  - labeled data (X, Y) from source population $(A = 1)$, and
  - unlabeled data $(X, \cdot)$ from target population $(A = 0)$

No informative PAC prediction set

Lemma

Suppose that X and Y are continuous. Under unknown covariate shift, if $\hat{C}$ is PAC, then under any data-generating distribution P^0 and for almost every y,

$$\Pr(y \notin \hat{C}(X) \mid A = 0) \leq \alpha_{\text{error}} + \alpha_{\text{conf}}.$$

Any PAC prediction set $\hat{C}$ is generally uninformative

- Consider $X \perp\!\!\!\perp Y$ and $Y \in \mathbb{R}$: might wish $\hat{C}(x) = (\hat{q}_{\alpha_{\text{error}}/2}, \hat{q}_{1-\alpha_{\text{error}}/2})$, but it is impossible to be PAC
- The following $\hat{C}$ is PAC but useless

$$\hat{C}(x) = \begin{cases} \mathbb{R} & \text{with probability } 1 - \alpha_{\text{error}} \\ \emptyset & \text{with probability } \alpha_{\text{error}} \end{cases}$$

Resort to asymptotic coverage guarantee

- *Asymptotically Probably Approximately Correct* (APAC) guarantee for prediction set $\hat{C}_n$:

$$\Pr\left(\Pr\left(Y \notin \hat{C}_n(X) \mid \text{training data}\right) \leq \alpha_{\text{error}}\right) \geq 1 - \alpha_{\text{conf}} - \mathrm{o}(1)$$

  as sample size $n \to \infty$.

- Interpretation: with high confidence level approaching $1 - \alpha_{\text{conf}}$, the coverage error rate of $\hat{C}_n$ is below α_{error}

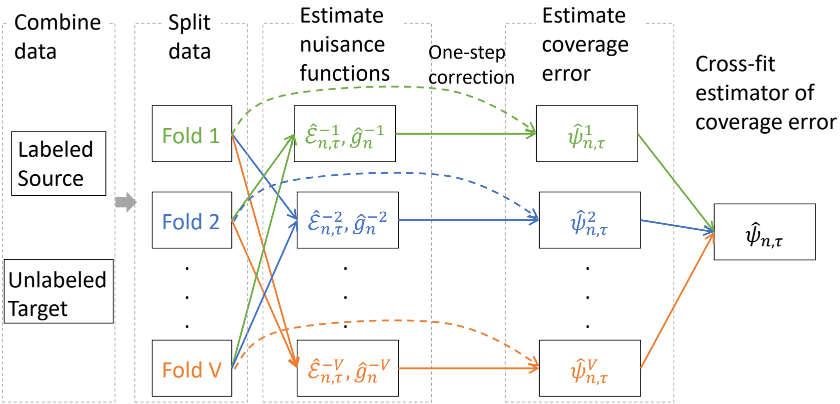
Proposed method: PredSet-1Step

- Given an arbitrary scoring function s, consider candidate prediction sets $C_\tau : x \mapsto \{y : s(x, y) \geq \tau\}$
- Examples of $s(x, y)$: estimated $\Pr(Y = y \mid X = x)$ or $f(Y = y \mid X = x)$ from held-out labeled data; $-|y - \hat{y}(x)|$ for a predictor $\hat{y}$ trained from held-out labeled data
- Using semiparametric efficiency theory, we construct an asymptotically efficient estimator (cross-fit one-step corrected estimator) $\hat{\psi}_{n,\tau}$ of the coverage error of C_τ in the target population:

$$\Pr(Y \notin C_\tau(X) \mid A = 0) =: \Psi_\tau(P^0)$$

- Construct a $(1 - \alpha_{\mathrm{conf}})$-confidence upper bound $\lambda_n(\tau)$ for $\Psi_\tau(P^0)$
- Select a threshold $\hat{\tau}_n$ from a grid $\mathcal{T}_n$ based on $\lambda_n(\tau)$

Flowchart of cross-fit one-step corrected estimator



Cross-fit one-step corrected estimator

1. Randomly split entire data set into V folds with index sets I_v $(v = 1, \ldots, V)$
2. For each fold v, estimate nuisance functions $(\mathcal{E}_{0,\tau}, g_0)$ with $(\hat{\mathcal{E}}_{n,\tau}^{-v}, \hat{g}_n^{-v})$ using data out of fold v

$$\mathcal{E}_{0,\tau}(x) := \Pr(Y \notin C_\tau(X) \mid X = x, A = 1)$$
$$g_0(x) := \Pr(A = 1 \mid X = x)$$

3. Let $\hat{\gamma}_n^v$ be the empirical proportion of $A = 1$ in fold v (estimator of $\Pr(A = 1)$)

Cross-fit one-step corrected estimator

4. For each fold v, compute one-step corrected estimator

$$\hat{\psi}^{v}_{n,\tau} := \underbrace{\frac{\sum_{i \in I_v} (1 - A_i) \hat{\mathcal{E}}^{-v}_{n,\tau}(X_i)}{\sum_{i \in I_v} (1 - A_i)}}_{\text{sample analogue of } \Psi_\tau(P^0)}$$

$$+ \underbrace{\frac{1}{|I_v|} \sum_{i \in I_v} \frac{A_i}{1 - \hat{\gamma}^{v}_{n}} \frac{1 - \hat{g}_n^{-v}(X_i)}{\hat{g}_n^{-v}(X_i)} [\mathbb{1}(Y_i \notin C_\tau(X_i)) - \hat{\mathcal{E}}^{-v}_{n,\tau}(X_i)]}_{\text{one-step correction}}.$$

5. Average over folds: $\hat{\psi}_{n,\tau} := \frac{1}{n} \sum_{v=1}^{V} |I_v| \hat{\psi}^{v}_{n,\tau}$.

Asymptotic efficiency

Theorem (Informal)

Under conditions, $\hat{\psi}_{n,\tau}$ *is an asymptotically efficient estimator of* $\Psi_\tau(P^0)$ *and*

$$\sqrt{n}(\hat{\psi}_{n,\tau} - \Psi_\tau(P^0)) \xrightarrow{d} \mathrm{N}\left(0, \sigma^2_{0,\tau}\right)$$

with $\sigma^2_{0,\tau} = \mathbb{E}_{P^0}[D_\tau(P^0)(O)^2]$ *where* $D_\tau(P^0)$ *is the efficient influence function.*

$(1-\alpha_{\mathrm{conf}})$-Wald confidence upper bound $\lambda_n(\tau)$ for $\Psi_\tau(P^0)$:

$$\lambda_n(\tau) = \hat{\psi}_{n,\tau} + z_{\alpha_{\mathrm{conf}}} \frac{\hat{\sigma}_{n,\tau}}{\sqrt{n}}$$

Selection of threshold

Select the threshold

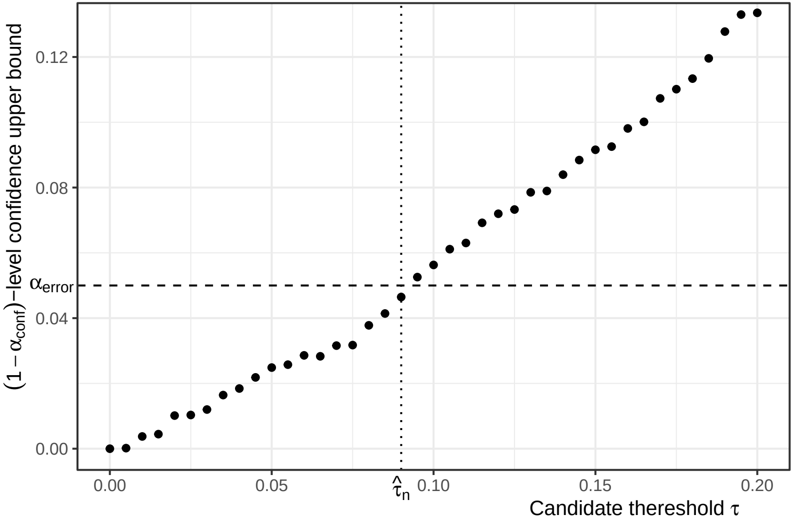
$$\hat{\tau}_n := \max\{\tau \in \mathcal{T}_n : \lambda_n(\tau') < \alpha_{\text{error}} \text{ for all } \tau' \in \mathcal{T}_n \text{ such that } \tau' \leq \tau\},$$

The largest candidate threshold such that all λ_n on the left hand side are below α_{error}. (Similar to Bates et al. [2021])

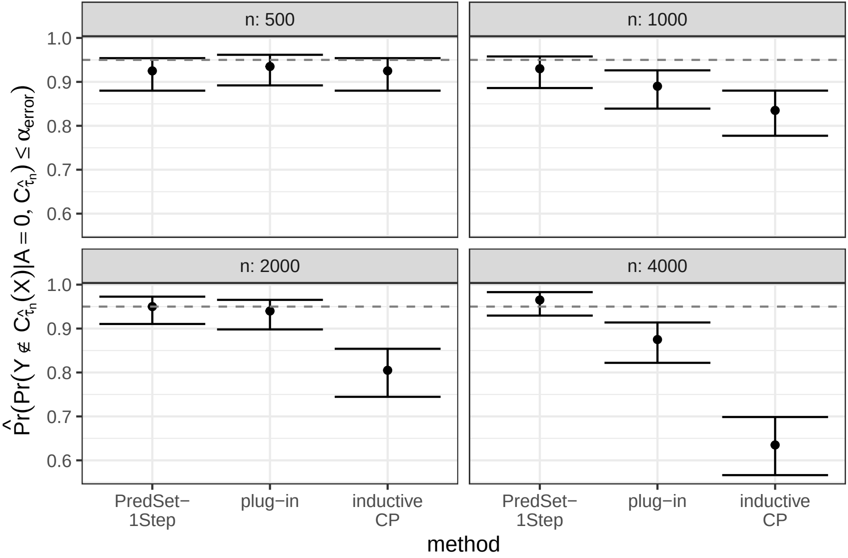
Theorem (Informal)

Under conditions, $C_{\hat{\tau}_n}$ is APAC.

Illustration of threshold selection



Simulation result



Analysis of HIV risk prediction data in South Africa

- Y: HIV infection
- Source population: urban and rural communities
- Target population: peri-urban communities with community HIV treatment coverage$\leq$15%
- Target coverage error $\alpha_{\text{error}} = 5\%$ (coverage$\geq$ 95%)
- Target confidence level $1 - \alpha_{\text{conf}} = 95\%$

Method	Empirical coverage	95% CI of coverage
PredSet-1Step	95.98%	94.83%–96.89%
Inductive CP	91.89%	90.35%–93.20%

Conclusion

- Prediction sets are useful to quantify uncertainty of prediction
- Unknown covariate shift is a common challenge
- We propose a method, PredSet-1step, to construct APAC prediction sets adaptive to unknown covariate shift

Acknowledgment

Collaborators:

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Eric Tchetgen Tchetgen

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arXiv preprint: `https://arxiv.org/abs/2203.06126` (will update soon)

R package available on Github.

Thank you!

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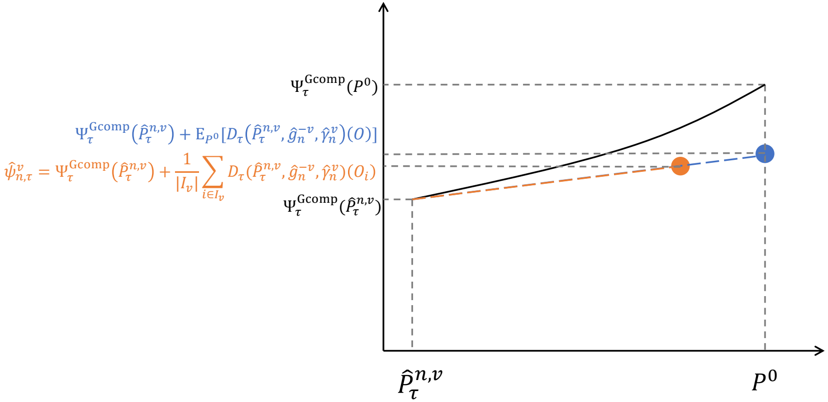
Intuition behind one-step correction: linear approximation



Without one-step correction, the naïve estimator $\Psi_\tau(\hat{P}_{n,\tau}^v)$ is generally asymptotically inefficient.

More technical results

Key condition for asymptotic efficiency of $\hat{\psi}_{n,\tau}$:

$$\|\hat{\mathcal{E}}_{n,\tau}^{-v} - \mathcal{E}_{0,\tau}\| \|\hat{g}_n^{-v} - g_0\| = \mathrm{o}_p(n^{-1/2})$$

Rate of $\mathrm{o}(1)$ term:

Theorem (Informal)

If the asymptotic variance is nonzero, the coverage probability $\mathrm{Pr}(\Psi_\tau(P^0) \leq \lambda_n(\tau))$ *equals*

$$1 - \alpha_{\mathrm{conf}} - \mathrm{O}\left(n^{1/4} \mathbb{E}_{P^0}[\|\hat{\mathcal{E}}_{n,\tau}^{-v} - \mathcal{E}_{0,\tau}\| \|\hat{g}_n^{-v} - g_0\|]^{1/2}\right)$$

The rate of the $\mathrm{o}(1)$ term is mainly determined by the product of convergence rates of the two nuisance function estimators.