Conformal Inference under Distributional Shift

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Conformal Prediction under Covariate Shift [Tibshirani et al., 2019]

Regression Setting: Observations $(X_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}$ for $i \in [n]$

Goal: Construct band $\hat{C}_n : \mathbb{R}^d \to \{\text{subsets of } \mathbb{R}\}$ based on the data $(X_i, Y_i)_{i=1}^n$ such that for a new (X_{n+1}, Y_{n+1})

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

Question: What can we do if the distribution of X_{n+1} is different?

Conformal Prediction

Notation:

- $Z_i = (X_i, Y_i)$, $Z_{1:n} = \{Z_1, \ldots, Z_n\}$, $Z_{-i} = Z_{1:n} \setminus \{Z_i\}$
- Score function S, small values of $S((x,y), Z)$ imply (x, y) conforms to Z
  - Example: $S((x,y), Z) = |y - \hat{\mu}(x)|$ for some regression function $\hat{\mu}$ trained on Z
- Nonconformity Scores:

$$V_i^{(x,y)} = S(Z_i, Z_{-i} \cup \{(x,y)\}), \quad V_{n+1}^{(x,y)} = S((x,y), Z_{1:n}),$$

- Let Quantile$(\beta; F)$ denote the β-th quantile of a distribution function F, i.e.

$$\text{Quantile}(\beta; F) = \inf\{z : F(z) \geq \beta\}$$

Use this to construct conformal confidence interval

$$\hat{C}_n(x) = \left\{ y \in \mathbb{R} : V_{n+1}^{(x,y)} \leq \text{Quantile}(1-\alpha; V_{1:n}^{(x,y)} \cup \{\infty\}) \right\}$$

Conformal Prediction Theorem

Theorem 1.

For exchangeable $(X_i, Y_i)_{i=1}^{n+1} \in \mathbb{R}^d \times \mathbb{R}$ *and any* $\alpha \in (0, 1)$, *then*

$$\hat{C}_n(x) = \left\{ y \in \mathbb{R} : V_{n+1}^{(x,y)} \leq \mathrm{Quantile}(1 - \alpha; V_{1:n}^{(x,y)} \cup \{\infty\}) \right\}$$

satisfies

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

If $V_1^{(X_{n+1}, Y_{n+1})}, \ldots, V_{n+1}^{(X_{n+1}, Y_{n+1})}$ *are distinct with probability* 1, *then the probability is upper bounded by* $1 - \alpha + 1/(n+1)$.

Covariate Shift

Consider the setting where the data are no longer exchangeable

$$
\begin{aligned}
(X_i, Y_i) &\overset{\text{i.i.d.}}{\sim} P = P_X \times P_{Y|X},\ i \in [n] \\
(X_{n+1}, Y_{n+1}) &\sim \tilde{P} = \tilde{P}_X \times P_{Y|X},\ \text{independently}
\end{aligned} \tag{1}
$$

Main Idea: If we preserve the conditional distribution $Y \mid X$ and we have knowledge of the covariate likelihood ratios $d\tilde{P}_X / dP_X$, can construct prediction band with marginal coverage

Covariate Shift

Idea: Use weights proportional to the likelihood ratio

- $w(X_i) = \frac{d\tilde{P}_X(X_i)}{dP_X(X_i)}$
- Conformal weights

$$p_i^w(x) = \frac{w(X_i)}{\sum_{j=1}^n w(X_j) + w(x)}, \ i \in [n]$$

$$p_{n+1}^w(x) = \frac{w(x)}{\sum_{j=1}^n w(X_j) + w(x)}$$

Covariate Shift Conformal Prediction Theorem

Theorem 2.

Under model (1)*, for any score function* S *and* $\alpha \in (0,1)$*, then*

$$\hat{C}_n(x) = \left\{ y \in \mathbb{R} : V_{n+1}^{(x,y)} \leq \text{Quantile}\left(1-\alpha; \sum_{i=1}^{n} p_i^w(x)\delta_{V_i^{(x,y)}} + p_{n+1}^w(x)\delta_\infty\right)\right\}$$

satisfies

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

Empirical Performance: Setup

Airfoil Dataset from UCI Machine Learning Repository

- $X \in \mathbb{R}^5$: log frequency, angle of attack, chord length, free-stream velocity, suction side log displacement thickness
- $Y \in \mathbb{R}$: scaled sound pressure of NASA airfoils
- $N = 1503$ observations
  - D_{pre}: 25% of the data to fit regression function μ_0
  - D_{train}: 25% of the data to compute residual quantiles for conformal prediction interval
  - D_{test}: 50% of the data for test set
  - D_{shift}: Sampled 25% from D_{test} with replacement with probabilities proportional to

    $$w(x) = \exp(x^\top \beta),\ \beta = (-1, 0, 0, 0, 1)$$

    Implies $d\tilde{P}_X \propto \exp(x^\top \beta) dP_X$[1]
- Simulations use 5000 random splits and $\alpha = 0.1$

[1] form of exponential tilting

Estimate Likehood Ratio

Consider $X_1, \ldots, X_n$ from D_{train} and $X_{n+1}, \ldots, X_{n+m}$ from D_{shift}

Procedure:

- Fit a classifier for (X_i, C_i) where $C_i = 0$ for $i = 1, \ldots, n$ and $C_i = 1$ for $i = n+1, \ldots, n+m$
- From Bayes Rule

$$\frac{\mathbb{P}[C = 1 \mid X = x]}{\mathbb{P}[C = 0 \mid X = x]} = \frac{\mathbb{P}[C = 1]}{\mathbb{P}[C = 0]} \frac{d\tilde{P}_X}{dP_X}(x)$$

- If $\hat{p}(x)$ is our estimate of $\mathbb{P}[C = 1 \mid X = x]$ from our classifier,

$$\hat{w}(x) = \frac{\hat{p}(x)}{1 - \hat{p}(x)}.$$

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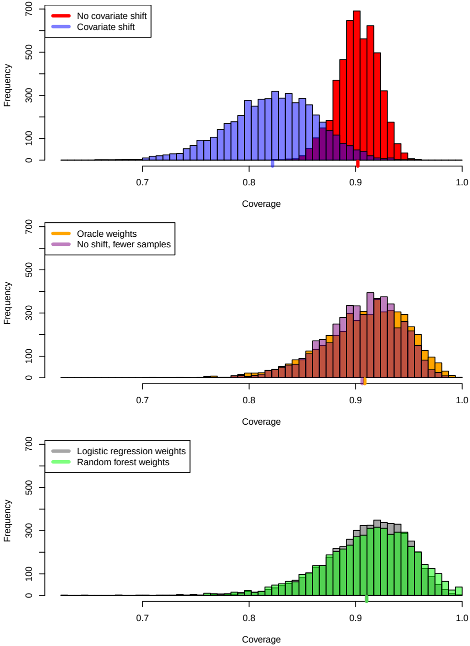
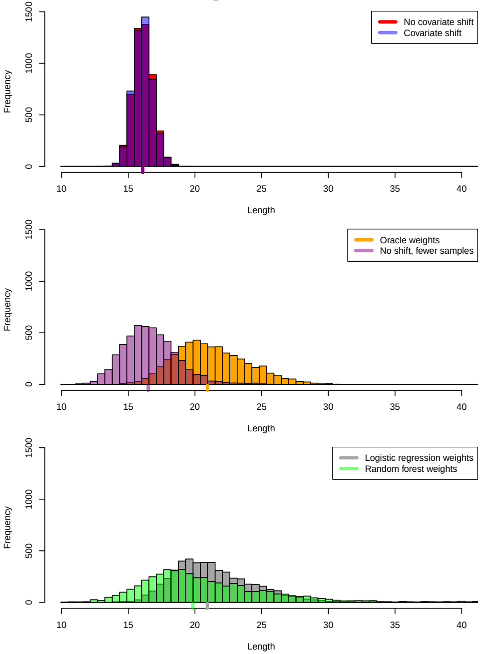
$$\hat{w}(x) = \frac{\hat{p}(x)}{1 - \hat{p}(x)}.$$

We do not need $\mathbb{P}[C = 1]$ since Theorem 2 holds when $w(x)$ is known up to a proportionality constant

Empirical Performance: Coverage



Empirical Performance: Length



Weighted Exchangeability

Definition 3.

Random variables $V_1, \ldots, V_n$ are weighted exchangeable with weight functions $w_1, \ldots, w_n$ if the density f of their joint distribution can be factorized as

$$f(v_1, \ldots, v_n) = \prod_{i=1}^{n} w_i(v_i) \cdot g(v_1, \ldots, v_n)$$

where g is any function that is independent on ordering, i.e.

$$g(v_{\sigma(1)}, \ldots, v_{\sigma(n)}) = g(v_1, \ldots, v_n)$$

for $\sigma \in S_n$.

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Example 4.

If $Z_i \overset{\text{ind.}}{\sim} P_i$ for $i \in [n]$ and P_i are absolutely continuous w.r.t. P_1, then $Z_1, \ldots, Z_n$ are weighted exchangeable with $w_1 \equiv 1$ and $w_i = dP_i/dP_1$.

Weighted Conformal Prediction

Theorem 5.

Let Z_i for $i \in [n+1]$ be weighted exchangeable random variables with weights $w_1, \ldots, w_{n+1}$. Let $V_i = S(Z_i, Z_{-i})$ for any score function S. Define

$$p_i^w(z_1, \ldots, z_{n+1}) = \frac{\sum_{\sigma:\sigma(n+1)=i} \prod_{j=1}^{n+1} w_j(z_{\sigma(j)})}{\sum_{\sigma} \prod_{j=1}^{n+1} w_j(z_{\sigma(j)})}$$

For $\alpha \in (0,1)$,

$$\mathbb{P}\left[V_{n+1} \leq \mathrm{Quantile}\left(1-\alpha; \sum_{i=1}^{n} p_i^w(Z_{1:n+1})\delta_{V_i} + p_{n+1}^w(Z_{1:n+1})\delta_{\infty}\right)\right] \geq 1-\alpha.$$

Weighted Conformal Prediction: Proof Sketch

Condition on event E_z where $\{Z_1, \ldots, Z_{n+1}\} = \{z_1, \ldots, z_{n+1}\}$ and $v_i = S(z_i, z_{-i})$

p_i^w is constructed so that from weighted exchangeability,

$$\mathbb{P}[V_{n+1} = v_i \mid E_z] = p_i^w(z_1, \ldots, z_{n+1}) \implies$$

$$V_{n+1} \mid E_z \sim \sum_{i=1}^{n+1} p_i^w(z_1, \ldots, z_{n+1}) \delta_{V_i} \implies$$

$$\mathbb{P}\left[V_{n+1} \leq \text{Quantile}\left(1-\alpha; \sum_{i=1}^{n} p_i^w(Z_{1:n+1})\delta_{V_i} + p_{n+1}^w(Z_{1:n+1})\delta_\infty\right)\right] \geq 1-\alpha.$$

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Problem Statement

Consider the more general online setting

Observations: $\{(X_r, Y_r)\}_{1 \leq r \leq t-1}$ and new covariate X_t where $(X_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}$

Goal: Construct prediction set $\hat{C}_t(X_t)$ for Y_t with marginal coverage

Challenge: No exchangeability or assumption on distribution of (X_i, Y_i), e.g. there may be distribution shifts for every observation rather than a train and shifted distribution

Prediction Set

Score Function: $S_t(X_t, y)$, e.g.

$$S_t(X_t, y) = |y - \hat{\mu}(X_t)|$$

Calibration Set: $\mathcal{D}_{\mathsf{cal}} \subseteq \{(X_r, Y_r)\}_{1 \leq r \leq t-1}$ distinct from data used to fit model

$$\hat{Q}_t(p) = \inf \left\{ s : \left(\frac{1}{|\mathcal{D}_{\mathsf{cal}}|} \sum_{(X_r, Y_r) \in \mathcal{D}_{\mathsf{cal}}} \mathbb{1}\{S(X_r, Y_r) \leq s\} \right) \geq p \right\}$$

Typical Prediction Set:

$$\hat{C}_t(X_t) = \{y : S_t(X_t, y) \leq \hat{Q}_t(1 - \alpha)\}$$

Miscoverage Rate

$$M_t(\alpha) = \mathbb{P}\left[S_t(X_t, Y_t) > \hat{Q}_t(1-\alpha)\right]$$

Ideally $M_t(\alpha) \approx \alpha$, but due to distributional shift this may be very different

Idea: There may be a different value $\alpha_t^\star \in [0,1]$ s.t. $M_t(\alpha_t^\star) = \alpha$

Question: Can we adaptively choose $\alpha_t^\star$ and use it as our cutoff?

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Answer: Yes! Field of Online Learning

Forecasters

Consider a Reasonably Young And Naive (RYAN) forecaster that uses the same α for every observation

- Large miscoverage rates $M_t(\alpha)$
- Cannot handle distribution shifts

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- Can statistically guarantee coverage on average even under arbitrary distributional shift

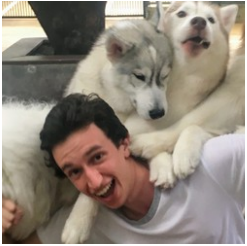

Figure: Ryan Brill, AMCS PhD Student

Forecasters

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- Large miscoverage rates $M_t(\alpha)$
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- Can statistically guarantee coverage on average even under arbitrary distributional shift

Figure: Bryan Frill, BRYAN forecaster

Adaptive Conformal Inference (ACI) [Gibbs and Candes, 2021]

The BRYAN forecaster monitors empirical miscoverage frequency and updates α_t

$$\hat{C}_t(\alpha_t) = \{y : S_t(X_t, y) \leq \hat{Q}_t(1 - \alpha_t)\}$$
$$\mathrm{err}_t = \mathbb{1}\{Y_t \notin \hat{C}_t(\alpha_t)\}$$

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Online Updates with step size $\gamma > 0$

$$\alpha_{t+1} = \alpha_t + \gamma(\alpha - \mathrm{err}_t)$$

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Online Updates with step size $\gamma > 0$

$$\alpha_{t+1} = \alpha_t + \gamma(\alpha - \mathrm{err}_t)$$

Smoothed Updates with $\sum_{s=1}^{t} w_s = 1$, e.g. $w_s \propto 0.95^{t-s}$

$$\alpha_{t+1} = \alpha_t + \gamma\left(\alpha - \sum_{s=1}^{t} w_s \mathrm{err}_s\right)$$

Coverage Guarantees I

Lemma 6.

With probability one, for all $t \geq 1$, $\alpha_t \in [-\gamma, 1+\gamma]$.

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With probability one, for all $t \geq 1$, $\alpha_t \in [-\gamma, 1+\gamma]$.

Proof.

For the sake of contradiction, assume $\alpha_{t+1} = \inf_i \alpha_i < -\gamma$. Then $\alpha_t < 0$ since

$$\alpha_{t+1} = \alpha_t + \gamma(\alpha - \mathrm{err}_t).$$

However if $\alpha_t < 0$, then

$$\alpha_t < 0 \implies \hat{Q}_t(1-\alpha_t) = \infty \implies$$
$$\mathrm{err}_t = 0 \implies \alpha_{t+1} = \alpha_t + \gamma(\alpha - \mathrm{err}_t) \geq \alpha_t$$

This is a contradiction, since $\alpha_{t+1} = \inf_i \alpha_i$ (similar argument for $\alpha_t \leq 1+\gamma$) □

Coverage Guarantees II

Theorem 7.

With probability one, for all $T \geq 1$,

$$\left| \frac{1}{T} \sum_{t=1}^{T} \mathrm{err}_t - \alpha \right| \leq \frac{\max(\alpha_1, 1 - \alpha_1) + \gamma}{T\gamma}$$

and

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} \mathrm{err}_t \overset{\text{a.s.}}{=} \alpha.$$

Coverage Guarantees II

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and

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} \mathrm{err}_t \overset{\text{a.s.}}{=} \alpha.$$

Proof.

$$\alpha_{T+1} = \alpha_1 + \sum_{t=1}^{T} \gamma(\alpha - \mathrm{err}_t) \implies \frac{\alpha_1 - \alpha_{T+1}}{\gamma T} = \frac{\sum_{t=1}^{T} \mathrm{err}_t - \alpha}{T}$$

Apply Lemma 6 to obtain desired inequality □

Empirical Performance: Market Volatility Coverage

Setup: Daily open prices for stock $\{P_t\}_{1\leq t\leq T}$, Returns $R_t = (P_t - P_{t-1})/P_{t-1}$

Goal: Prediction set for volatility $V_t = R_t^2$ with $\alpha = 0.1$

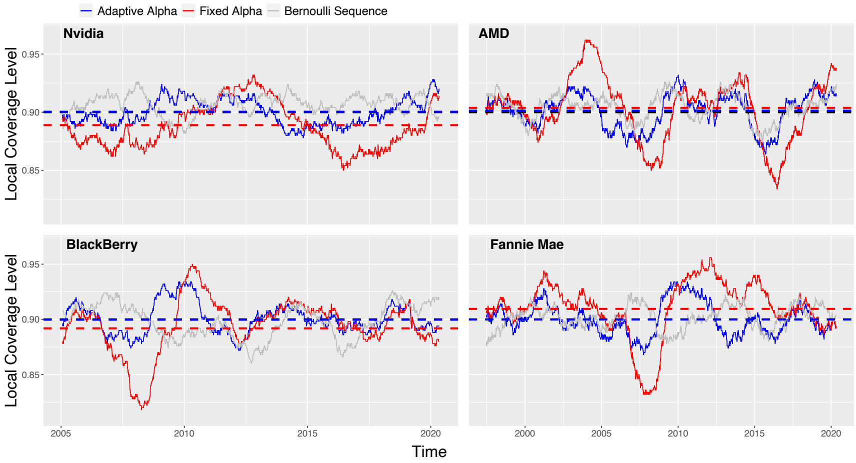
Local Coverage Frequency:

$$\mathsf{localCov}_t = 1 - \frac{1}{500}\sum_{r=t-250+1}^{t+250} \mathrm{err}_r$$

Bernoulli Baseline: $\{I_t\}_{1\leq t\leq T}$ i.i.d. Bernoulli(0.1)

$$1 - \frac{1}{500}\sum_{r=t-250+1}^{t+250} I_r$$

Empirical Performance: Market Volatility Coverage



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A Standard Causal Inference Setting [Lei and Candes, 2021]

Setup/Notation:

- n subjects
- T_i the binary treatment indicator
- $(Y_i(1), Y_i(0))$ the potential outcomes under treatment and control
- X_i the vector of covariates
- Assume $(Y_i(1), Y_i(0), T_i, X_i) \overset{iid}{\sim} (Y(1), Y(0), T, X)$ (superpopulation)

Under the stable unit treatment value assumption, the observed dataset comprises triples $(Y_i^{\text{obs}}, T_i, X_i)$ where

$$Y_i^{\text{obs}} = T_i Y_i(1) + (1 - T_i) Y_i(0)$$

The individual treatment effect τ_i is defined as $Y_i(1) - Y_i(0)$

Goal: Construct $\hat{C}_1 : \mathbb{R}^d \to \{\text{subsets of } \mathbb{R}\}$ such that

$$\mathbb{P}\left[Y(1) \in \hat{C}_1(X)\right] \geq 1 - \alpha$$

Connection to Weighted Conformal Prediction

Strong Ignorability: $(Y(1), Y(0)) \perp\!\!\!\perp T | X$

Observe that in the treated group, we have

$$\begin{aligned} P(X, Y^{\text{obs}} | T = 1) &= P(X | T = 1) P(Y^{\text{obs}} | X, T = 1) \\ &= P(X | T = 1) P(Y(1) | X, T = 1) \\ &= P(X | T = 1) P(Y(1) | X) \end{aligned}$$

From the treated group, we observe data from $P_{X|T=1} \times P_{Y(1)|X}$ but we want prediction regions for $P_X \times P_{Y(1)|X}$. This is exactly the setting from weighted conformal prediction with weights $dP_X / dP_{X|T=1} \propto 1/e(X)$ where $e(X) := \mathbb{P}[T = 1 | X]$ is the propensity score.

Connection to Weighted Conformal Prediction

If we were instead interested in prediction regions for $P_{X|T=1} \times P_{Y(1)|T=1,X}$, the weights would simply be 1. If we were instead interested in prediction regions for $P_{X|T=0} \times P_{Y(1)|T=0,X}$, the weights would be $dP_{X|T=0}/dP_{X|T=1} \propto (1 - e(X))/e(X)$. The below table summarizes weights for specific settings of interest:

Table 1. Summary of weight functions for different inferential targets

Inferential type	ATE	ATT	ATC	General
$w_1(x)$	$1/e(x)$	1	$(1-e(x))/e(x)$	$(dQ/dP)(x)/e(x)$
$w_0(x)$	$1/(1-e(x))$	$e(x)/(1-e(x))$	1	$(dQ/dP)(x)/(1-e(x))$

The weighted conformal framework requires the weights to be known; in practice they are estimated as the propensity score is unknown.

Algorithm

The authors propose to use a weighted version of conformalized quantile regression. The algorithm is below:

Algorithm 1 Weighted split-CQR

Input: level α, data $\mathcal{Z} = (X_i, Y_i)_{i \in \mathcal{I}}$, testing point x, function $\hat{q}_\beta(x; \mathcal{D})$ to fit β-th conditional quantile and function $\hat{w}(x; \mathcal{D})$ to fit the weight function at x using $\mathcal{D}$ as data

Procedure:

1: Split $\mathcal{Z}$ into a training fold $\mathcal{Z}_{\text{tr}} \triangleq (X_i, Y_i)_{i \in \mathcal{I}_{\text{tr}}}$ and a calibration fold $\mathcal{Z}_{\text{ca}} \triangleq (X_i, Y_i)_{i \in \mathcal{I}_{\text{ca}}}$

2: For each $i \in \mathcal{I}_{\text{ca}}$, compute the score $V_i = \max\{\hat{q}_{\alpha_{\text{lo}}}(X_i; \mathcal{Z}_{\text{tr}}) - Y_i, Y_i - \hat{q}_{\alpha_{\text{hi}}}(X_i; \mathcal{Z}_{\text{tr}})\}$

3: For each $i \in \mathcal{I}_{\text{ca}}$, compute the weight $W_i = \hat{w}(X_i; \mathcal{Z}_{\text{tr}}) \in [0, \infty)$

4: Compute the normalized weights $\hat{p}_i(x) = \frac{W_i}{\sum_{i \in \mathcal{I}_{\text{ca}}} W_i + \hat{w}(x; \mathcal{Z}_{\text{tr}})}$ and $\hat{p}_\infty(x) = \frac{\hat{w}(x; \mathcal{Z}_{\text{tr}})}{\sum_{i \in \mathcal{I}_{\text{ca}}} W_i + \hat{w}(x; \mathcal{Z}_{\text{tr}})}$

5: Compute $\eta(x)$ as the $(1-\alpha)$-th quantile of the distribution $\sum_{i \in \mathcal{I}_{\text{ca}}} \hat{p}_i(x) \delta_{V_i} + \hat{p}_\infty(x) \delta_\infty$

Output: $\hat{C}(x) = [\hat{q}_{\alpha_{\text{lo}}}(x; \mathcal{Z}_{\text{tr}}) - \eta(x), \hat{q}_{\alpha_{\text{hi}}}(x; \mathcal{Z}_{\text{tr}}) + \eta(x)]$

Validity Theorem

Theorem 8.

Let $(X_i, Y_i) \overset{\text{i.i.d.}}{\sim} (X, Y) \sim P_X \times P_{Y|X}$ *and* Q_X *be another distribution. Set* $N = |\mathcal{Z}_{\mathrm{tr}}|$ *and* $n = |\mathcal{Z}_{\mathrm{ca}}|$. *Further, let* $\hat{q}_{\beta,N}(x)$ *be an estimate of the* β*-th conditional quantile* $q_\beta(x)$ *of* $Y \mid X = x, \hat{w}_N(x)$ *be an estimate of* $w(x) = (dQ_X/dP_X)(x)$, *and* $\hat{C}_{N,n}(x)$ *be the conformal interval resulting from Algorithm 1. Then*

$$\mathbb{P}_{(X,Y)\sim Q_X \times P_{Y|X}}\left(Y \in \hat{C}_{N,n}(X)\right) \geq 1 - \alpha - \frac{1}{2}\mathbb{E}_{X\sim P_X}\left|\hat{w}_N(X) - w(X)\right|.$$

Proof Intuition

For $\mathcal{E}(V)$ the set of unordered V and for $\mathcal{E}\left(v^*\right)$ a particular set of v^*, $\left(V_{n+1} \mid \mathcal{E}(V)=\mathcal{E}\left(v^*\right), \mathcal{Z}_{\mathrm{tr}}\right) \sim \sum_{i=1}^{n+1} p_i\left(X_{n+1}\right) \delta_{v_i^*}$

Next, define a measure $\tilde{Q}_X$ such that $\tilde{Q}_X=\hat{w}(x) d P_X$
$\left(\tilde{V}_{n+1} \mid \mathcal{E}(\tilde{V})=\mathcal{E}\left(v^*\right), \mathcal{Z}_{\mathrm{tr}}\right) \sim \sum_{i=1}^{n+1} \hat{p}_i\left(\tilde{X}_{n+1}\right) \delta_{v_i^*}$

There is a lemma that states
$d_{\mathrm{TV}}\left(Q_X \times P_{Y \mid X}, \tilde{Q}_X \times P_{Y \mid X}\right)=d_{\mathrm{TV}}\left(Q_X, \tilde{Q}_X\right)$

$$
\begin{aligned}
\left|\mathbb{P}\left(Y_{n+1} \in \hat{C}\left(X_{n+1}\right) \mid \mathcal{Z}_{\mathrm{tr}}, \mathcal{Z}_{\mathrm{ca}}\right)-\mathbb{P}\left(\tilde{Y}_{n+1} \in \hat{C}\left(\tilde{X}_{n+1}\right) \mid \mathcal{Z}_{\mathrm{tr}}, \mathcal{Z}_{\mathrm{ca}}\right)\right| & \\
\leq d_{\mathrm{TV}}\left(Q_X, \tilde{Q}_X\right) \ldots & \\
\mathbb{P}\left(Y_{n+1} \in \hat{C}\left(X_{n+1}\right) \mid \mathcal{Z}_{\mathrm{tr}}\right) \geq 1-\alpha-d_{\mathrm{TV}}\left(Q_X, \tilde{Q}_X\right) \ldots & \\
\mathbb{P}\left(Y_{n+1} \in \hat{C}\left(X_{n+1}\right)\right) \geq 1-\alpha-\frac{1}{2} \mathbb{E}_{X \sim P_X}|\hat{w}(X)-w(X)| &
\end{aligned}
$$

Simulation Study

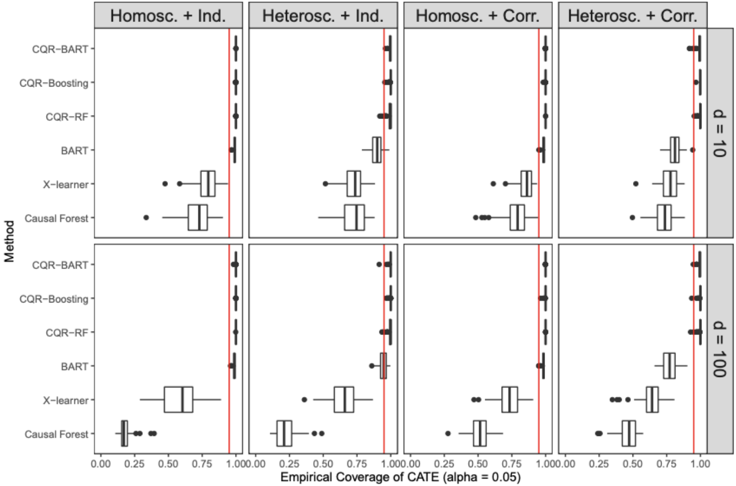
Setup: Generate 100 datasets of 1000 subjects and 10000 test subjects. Compare weighted CQR with BART, Causal Forest, and X-Learner on marginal coverage of the CATE, defined as

$$(1/n_{\text{test}}) \sum_{i=1}^{n_{\text{test}}} \mathbf{1}(\tau(X_i) \in \hat{C}_{ITE}(X_i))$$

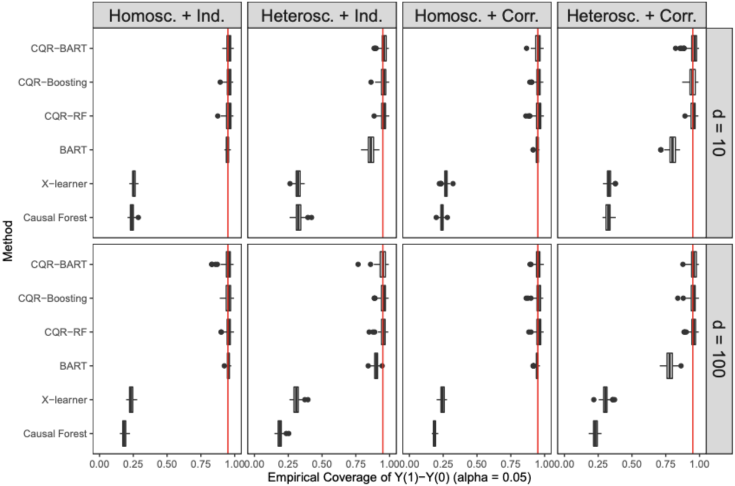
and marginal coverage of the ITE, defined as

$$(1/n_{\text{test}}) \sum_{i=1}^{n_{\text{test}}} \mathbf{1}(Y_i(1) - Y_i(0) \in \hat{C}_{ITE}(X_i))$$

Simulation Results



Simulation Results



Violation of Strong Ignorability [Jin et al., 2021]

Strong ignorability is typically an untenable assumption. Assume instead that for some unmeasured confounder U, we have

$$(Y(1), Y(0)) \perp\!\!\!\perp T | X, U$$

Without further assumptions, cannot proceed. Instead, bound the "strength" of the unmeasured confounder.

Definition 9.

A distribution $\mathbb{P}$ over $(X, U, T, Y(0), Y(1))$ satisfies the marginal Γ-selection condition if for $\mathbb{P}$-almost all x and u

$$1/\Gamma \leq \frac{\mathbb{P}(T = 1 | X = x, U = u)/\mathbb{P}(T = 0 | X = x, U = u)}{\mathbb{P}(T = 1 | X = x)/\mathbb{P}(T = 0 | X = x)} \leq \Gamma$$

Goal: Construct $\hat{C}_1 : \mathbb{R}^d \to \{\text{subsets of } \mathbb{R}\}$ such that

$$\mathbb{P}\left[Y(1) \in \hat{C}_1(X, \Gamma)\right] \geq 1 - \alpha$$

for all $\mathbb{P}^{\text{sup}}$ that satisfy the Γ-marginal selection.

A Review of Weighted Conformal Inference

Suppose we have (X_i, Y_i) from distribution $\mathbb{P}$ and a test point (X_{n+1}, Y_{n+1}) from a different distribution $\tilde{\mathbb{P}}$, where $\tilde{\mathbb{P}}$ is within a bounded distance of $\mathbb{P}$ in that it belongs to the set

$$\{\tilde{\mathbb{P}} : l(x) \leq \frac{d\tilde{\mathbb{P}}}{d\mathbb{P}}(x, y) \leq u(x)\}$$

If we assume $w(x, y) = \frac{d\tilde{\mathbb{P}}}{d\mathbb{P}}(x, y)$ is known exactly, we can directly apply the results of Tibshirani et al. [2019].

- Non-conformity score V
- $p_i^w(x, y) := \frac{w(X_i, Y_i)}{\sum_{j=1}^n w(X_j, Y_j) + w(x, y)}, i = 1, \ldots, n,$
  $p_{n+1}^w(x, y) := \frac{w(x, y)}{\sum_{j=1}^n w(X_j, Y_j) + w(x, y)}$
- $\widehat{C}\left(X_{n+1}\right) = \left\{y : V\left(X_{n+1}, y\right) \leq \widehat{V}_{1-\alpha}(y)\right\}$ where $\widehat{V}_{1-\alpha}(y) =$ Quantile $\left(1 - \alpha, \sum^n p_i^w\left(X_{n+1}, y\right) \cdot \delta_{V_i} + p_{n+1}^w\left(X_{n+1}, y\right) \cdot \delta_{\infty}\right)$

Robust Weighted Procedure

- Let $V_{[1]} \leq \ldots \leq V_{[n]}$ be a reordering of the conformity scores on the calibration set
- Let $\hat{l}(x)$ and $\hat{u}(x)$ be estimated upper and lower bounds on $w(x, y)$
- Define $l_i = \hat{l}(X_i)$ and $u_i = \hat{u}(X_i)$

Take the prediction interval $\widehat{C}\left(X_{n+1}\right) = \left\{y : V\left(X_{n+1}, y\right) \leq \widehat{V}_{k^*}\right\}$ where

$k^* = \min\{k : \widehat{F}(k) \geq 1 - \alpha\}, \quad \widehat{F}(k) = \frac{\sum_{i=1}^{k} \ell_{[i]}}{\sum_{i=1}^{k} \ell_{[i]} + \sum_{i=k+1}^{n} u_{[i]} + u_{n+1}}$

The $\widehat{F}(k)$ can be shown to be the solution to

$$\operatorname{minimize}_W \frac{\sum_{i=1}^{k} W_{[i]}}{\sum_{i=1}^{n} W_i + W_{n+1}}$$

subject to $\widehat{\ell}\left(X_i\right) \leq W_i \leq \widehat{u}\left(X_i\right), \quad \forall i \in \mathcal{D}_{\text{calib}} \cup \{n+1\}$

Robust Weighted Procedure

The procedure is summarized below:

Algorithm 1 Robust conformal prediction: the marginal procedure

Input: Calibration data $\mathcal{D}_{\text{calib}}$, bounds $\widehat{\ell}(\cdot)$, $\widehat{u}(\cdot)$, non-conformity score function $V\colon \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, test covariate x, target level $\alpha \in (0,1)$.

1: For each $i \in \mathcal{D}_{\text{calib}}$, compute $V_i = V(X_i, Y_i)$
2: For each $i \in \mathcal{D}_{\text{calib}}$, compute $\ell_i = \widehat{\ell}(X_i)$ and $u_i = \widehat{u}(X_i)$.
3: Compute $u_{n+1} = \widehat{u}(x)$.
4: For each $1 \le k \le n$, compute $\widehat{F}(k)$ as in (8).
5: Compute $k^* = \min\{k\colon \widehat{F}(k) \ge 1 - \alpha\}$.

Output: Prediction set $\widehat{C}(x) = \{y\colon V(x,y) \le V_{[k^*]}\}$.

with the guarantee ...

Robust Weighted Procedure

Theorem 10.

Assume $(X_i, Y_i) i.i.d. \sim \mathbb{P}$*, and the independent test point* $(X_{n+1}, Y_{n+1}) \sim \tilde{\mathbb{P}}$ *has likelihood ratio* $w(x,y) = \frac{d\tilde{\mathbb{P}}}{d\mathbb{P}}(x,y)$*. Then for any target level* $\alpha \in (0,1)$*, the output of Algorithm 1 satisfies*

$$\tilde{P}(Y_{n+1} \in \widehat{C}(X_{n+1}) \geq 1 - \alpha - \hat{\Delta}$$

where $\widehat{\Delta} =$
$\|1/\widehat{\ell}(X)\|_q \cdot \left(\left\| (\widehat{\ell}(X) - w(X,Y))_+ \right\|_p + \|(\widehat{u}(X) - w(X,Y))_-\|_p \right.$
$\left. + \frac{1}{n} \left\| w(X,Y)^{1/p} \cdot (\widehat{u}(X) - w(X,Y))_- \right\|_p \right)$

Bounding the Likelihood Ratio

Under the Γ-selection condition, it is possible to show the following:

Lemma 11.

Suppose a distribution $\mathbb{P}$ *over* $(X, U, T, Y(0), Y(1))$ *satisfies the marginal* Γ*-selection condition. Then for any* $t \in \{0, 1\}$ *it holds for* $\mathbb{P}$*-almost all* x, y *that*

$$1/\Gamma \leq \frac{dP_{Y(t)|X,T=t}}{dP_{Y(t)|X,T=1-t}}(x, y) \leq \Gamma$$

Note that the observed data always factors as $\mathbb{P}_{X,Y(t)|T=t}$. We may be interested in $\mathbb{P}_{X,Y(t)}$. Bayes rule shows

$$\frac{d\mathbb{P}_{X,Y(1)}}{d\mathbb{P}_{X,Y(1)|T=1}} = \mathbb{P}(T = 1) \times \left(1 + \frac{dP_{Y(1)|X,T=1}}{dP_{Y(1)|X,T=0}} \times \frac{e(X)}{1 - e(X)}\right)$$

Bounding the Likelihood Ratio

Applying the Lemma, we get that

$$\mathbb{P}(T=1)\times\left(1+1/\Gamma\times\frac{e(X)}{1-e(X)}\right)\leq\frac{d\mathbb{P}_{X,Y(1)}}{d\mathbb{P}_{X,Y(1)|T=1}}$$
$$\leq\mathbb{P}(T=1)\times\left(1+\Gamma\times\frac{e(X)}{1-e(X)}\right)$$

So the likelihood ratio of what we are interested in and what we have observed has been bounded by a function of X and Γ.

Counterfactual	Bound	ATE-type	ATT-type	ATC-type	General
$Y(1)$	$\ell(x)$	$p_1\cdot\left(1+\frac{1}{\Gamma\cdot r(x)}\right)$	1	$\frac{p_1}{p_0}\cdot\left(\frac{1}{\Gamma\cdot r(x)}\right)$	$p_1\cdot\frac{\mathrm{d}\mathbb{Q}_X}{\mathrm{d}\mathbb{P}_X}(x)\cdot\left(1+\frac{1}{\Gamma\cdot r(x)}\right)$
	$u(x)$	$p_1\cdot\left(1+\frac{\Gamma}{r(x)}\right)$	1	$\frac{p_1}{p_0}\cdot\frac{\Gamma}{r(x)}$	$p_1\cdot\frac{\mathrm{d}\mathbb{Q}_X}{\mathrm{d}\mathbb{P}_X}(x)\cdot\left(1+\frac{\Gamma}{r(x)}\right)$
$Y(0)$	$\ell(x)$	$p_0\cdot\left(1+\frac{r(x)}{\Gamma}\right)$	$\frac{p_0}{p_1}\cdot\frac{r(x)}{\Gamma}$	1	$p_0\cdot\frac{\mathrm{d}\mathbb{Q}_X}{\mathrm{d}\mathbb{P}_X}(x)\cdot\left(1+\frac{r(x)}{\Gamma}\right)$
	$u(x)$	$p_0\cdot\left(1+\Gamma\cdot r(x)\right)$	$\frac{p_0}{p_1}\cdot\Gamma\cdot r(x)$	1	$p_0\cdot\frac{\mathrm{d}\mathbb{Q}_X}{\mathrm{d}\mathbb{P}_X}(x)\cdot\left(1+\Gamma\cdot r(x)\right)$

Table 1: Summary of the upper and lower bounds of the likelihood ratio for different inferential targets. For $t\in\{0,1\}$, $p_t=\mathbb{P}(T=t)$ and $r(x)=e(x)/(1-e(x))$ is the odds ratio of the propensity score. The training distribution for $Y(t)$ is always $\mathbb{P}_{X,Y(t)\,|\,T=t}$. For target distributions, ATE-type refers to $\mathbb{P}_{X,Y(t)}$; ATT-type refers to $\mathbb{P}_{X,Y(t)\,|\,T=1}$; ATC-type refers to $\mathbb{P}_{X,Y(t)\,|\,T=0}$; General refers to $\mathbb{Q}_X\times\mathbb{P}_{Y(t)\,|\,X}$.

Proof Sketch of Lemma

By rearranging the Γ-selection condition and using Bayes rule, we can derive $\frac{1}{\Gamma} \leq \frac{\mathrm{d}\mathbb{P}_{U|X,T=1}}{\mathrm{d}\mathbb{P}_{U|X,T=0}}(u,x) \leq \Gamma$ for almost every u, x. Also, for any measurable B,

$$\begin{aligned}\mathbb{P}(Y(1) \in B, T = t \mid X) &= \mathbb{E}\left[\mathbb{E}\left[\mathbf{1}_{\{Y(1)\in B\}}\mathbf{1}_{\{T=t\}} \mid X, U\right] \mid X\right] \\ &= \mathbb{E}\left[\mathbb{E}\left[\mathbf{1}_{\{Y(1)\in B\}} \mid X, U\right] \cdot \mathbb{E}\left[\mathbf{1}_{\{T=t\}} \mid X, U\right] \mid X\right]\end{aligned}$$

Rearranging the Γ-selection condition, we have

$$\begin{aligned}\frac{1}{\Gamma} \cdot \mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X, U\right] \cdot \frac{\mathbb{E}\left[\mathbf{1}_{\{T=1\}} \mid X\right]}{\mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X\right]} &\leq \mathbb{E}\left[\mathbf{1}_{\{T=1\}} \mid X, U\right] \\ &\leq \Gamma \cdot \mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X, U\right] \cdot \frac{\mathbb{E}\left[\mathbf{1}_{\{T=1\}} \mid X\right]}{\mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X\right]}\end{aligned}$$

Proof Sketch Continued

Multiplying the previous by $\mathbb{E}[\mathbf{1}\{Y(1) \in B\}|X, U]$ and taking expectation conditional on X,

$$\begin{aligned}
&\frac{1}{\Gamma} \cdot \mathbb{P}(Y(1) \in B, T = 0 \mid X) \cdot \frac{\mathbb{E}\left[\mathbf{1}_{\{T=1\}} \mid X\right]}{\mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X\right]} \\
&\quad \leq \mathbb{P}(Y(1) \in B, T = 1 \mid X) \\
&\quad \leq \Gamma \cdot \mathbb{P}(Y(1) \in B, T = 0 \mid X) \cdot \frac{\mathbb{E}\left[\mathbf{1}_{\{T=1\}} \mid X\right]}{\mathbb{E}\left[\mathbf{1}_{\{T=0\}} \mid X\right]}
\end{aligned}$$

$$\frac{1}{\Gamma} \cdot \frac{1 - e(x)}{e(x)} \leq \frac{\mathbb{P}(Y(1) \in B, T = 0 \mid X = x)}{\mathbb{P}(Y(1) \in B, T = 1 \mid X = x)} \leq \Gamma \cdot \frac{1 - e(x)}{e(x)}$$

Note

$$\frac{\mathbb{P}(Y(1) \in B \mid X = x, T = 1)}{\mathbb{P}(Y(1) \in B \mid X = x, T = 0)} = \frac{\mathbb{P}(Y(1) \in B, T = 1 \mid X = x)}{\mathbb{P}(Y(1) \in B, T = 0 \mid X = x)} \cdot \frac{1 - e(x)}{e(x)}$$

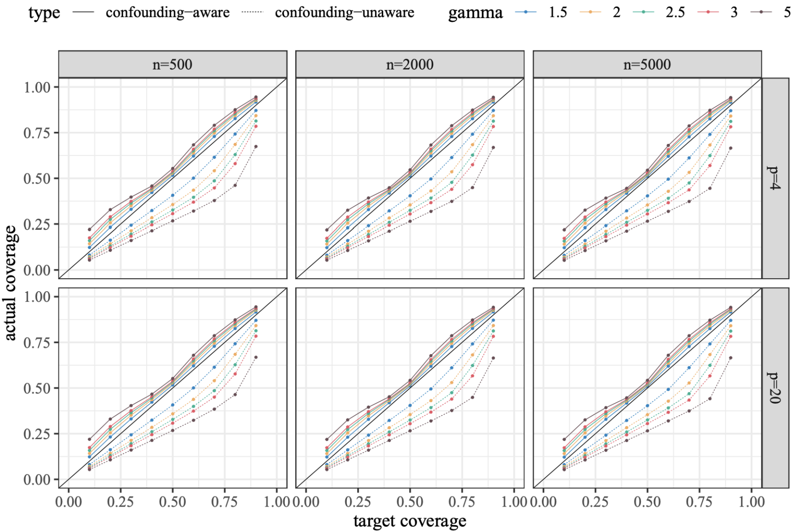
Conclude $\frac{1}{\Gamma} \leq \frac{d\mathbb{P}_{Y(1)|X,T=1}}{d\mathbb{P}_{Y(1)|X,T=0}}(x, y) \leq \Gamma$.

Simulation Study

Setup: Over sample sizes 500,2000,5000 and dimension 4 and 20, generate treatment with different confounding levels.

$$
\begin{aligned}
&X \sim \mathsf{Unif}[0,1]^p \\
&U|X \sim N(0, 1 + 0.5 \times (2.5X_1)^2) \\
&Y(1) = \beta^T X + U \\
&e(x) = \mathsf{logit}(\beta^T x) \\
&e(x,u) = a(x)\mathbf{1}\{|u| > t(x)\} + b(x)\mathbf{1}\{|u| \le t(x)\} \\
&a(x) = \frac{e(x)}{e(x) + \Gamma(1 - e(x))}, b(x) = \frac{e(x)}{e(x) + 1/\Gamma(1 - e(x))}
\end{aligned}
$$

Simulation Results



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