Introduction of Conformal Inference

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Outline

Objective of conformal inference

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- Constructing a prediction interval $C \subseteq \mathbb{R}^d \times \mathbb{R}$ based on $Z_1, \ldots, Z_n$ with the property that

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

A simple exercise

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Suppose we have positive i.i.d random variables $R_1, \cdots, R_n, R_{n+1}$. Let $Q_{1-\alpha}$ denote the empirical $1-\alpha$ quantile for $\{R_1, \cdots, R_n\}$, what is approximate value of $\mathbb{P}(R_{n+1} \leq Q_{1-\alpha})$?

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Answer: Consider ordered statisitics for $n+1$ R_i

$$R_{(1)}, R_{(2)}, R_{(3)}, \cdots, R_{(n)}, R_{(n+1)}$$

$$\mathbb{P}(R_{n+1} \leq Q_{1-\alpha}) \approx \mathbb{P}(R_{n+1} \text{ rank lower than } (1-\alpha)(n+1)) \approx 1-\alpha \quad (2)$$

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Inverse the empirical CDF: $\text{Quantile}\left(1-\alpha; \frac{1}{n}\sum_{i=1}^{n} \delta_{R_i}\right)$
Remark: relax i.i.d to exchangeable.

Construction of conformal prediction set

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$$1-\alpha \approx \mathbb{P}(R_{n+1} \leq Q_{1-\alpha}) = \mathbb{P}(|Y_{n+1} - \hat{\mu}(X_{n+1})| \leq Q_{1-\alpha})$$

$$\Rightarrow \mathbb{P}(Y_{n+1} \in [\hat{\mu}(X_{n+1}) - Q_{1-\alpha}, \hat{\mu}(X_{n+1}) + Q_{1-\alpha}]) \approx 1-\alpha$$

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- [LGR+18] Define $C_{\text{split}}(x) = [\widehat{\mu}(x) - Q_{1-\alpha}, \widehat{\mu}(x) + Q_{1-\alpha}]$

$$1-\alpha \leq \mathbb{P}\left(Y_{n+1} \in C_{\text{split}}(X_{n+1})\right) \leq 1-\alpha + \frac{2}{n+2}$$

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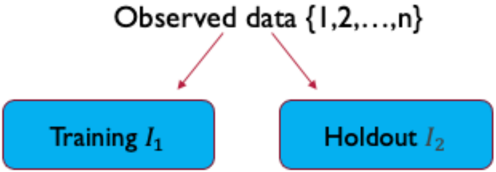

For **any** regression algorithm $\mathcal{A}$

$\widehat{\mu} = \mathcal{A}(\{(X_i, Y_i) : i \in \mathcal{I}_1\})$

$R_i = \left|Y_i - \widehat{\mu}(X_i)\right|, i \in \mathcal{I}_2$

$Q_{1-\alpha}$ is $(1-\alpha)(|\mathcal{I}_2| + 1)$ quantile of $\{R_i : i \in \mathcal{I}_2\}$

Return $C_{\text{split}}(x) = [\widehat{\mu}(x) - Q_{1-\alpha}, \widehat{\mu}(x) + Q_{1-\alpha}]$, for all $x \in \mathbb{R}^d$

Remark on conformal prediction set

$$C_{\text{split}}(X_{n+1}) = [\widehat{\mu}(X_{n+1}) - Q_{1-\alpha}, \widehat{\mu}(X_{n+1}) + Q_{1-\alpha}]$$

- Marginal coverage: $\mathbb{P}$ is over joint distribution of (X, Y),i.e. $\mathbb{P}_{(X,Y)}$

$$1 - \alpha \leq \mathbb{P}_{(X,Y)}\left(Y_{n+1} \in C_{\text{split}}(X_{n+1})\right) \leq 1 - \alpha + \frac{2}{|\mathcal{I}_2| + 2}$$

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Much stronger property

$$\mathbb{P}(Y_{n+1} \in C(x) \mid X_{n+1} = x) \geq 1 - \alpha \text{ for all } x \in \mathbb{R}^d$$

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- Problem of C_{split}: Constant CI width equal to $2Q_{1-\alpha}$ for any X_{n+1}, solution: use training data to fit an local variability $\hat{\rho}(x)$

$$R_{n+1} = \frac{\left|Y_{n+1} - \widehat{\mu}(X_{n+1})\right|}{\widehat{\rho}(X_{n+1})}, \quad R_i = \frac{\left|Y_i - \widehat{\mu}(X_i)\right|}{\widehat{\rho}(X_i)}, i \in \mathcal{I}_2$$

$$C_{\text{split}}^{\text{local}}(X_{n+1}) = [\widehat{\mu}(X_{n+1}) - \widehat{\rho}(X_{n+1})Q_{1-\alpha}, \widehat{\mu}(X_{n+1}) + \widehat{\rho}(X_{n+1})Q_{1-\alpha}]$$

Alternative method: Conformal quantile regression [RPC19]

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- Training $\mathcal{I}_1$, holdout $\mathcal{I}_2$. For **any quantile** regression algorithm $\mathcal{A}$
  $\widehat{q} = \mathcal{A}(\{(X_i, Y_i) : i \in \mathcal{I}_1\})$
  $R_i^{\mathrm{CQR}} = \max\left\{\hat{q}_{\alpha/2}(X_i) - Y_i, Y_i - \hat{q}_{1-\alpha/2}(X_i)\right\}, i \in \mathcal{I}_2$
  $Q_{1-\alpha}$ is $(1-\alpha)(|\mathcal{I}_2|+1)$ quantile of $\left\{R_i^{\mathrm{CQR}} : i \in \mathcal{I}_2\right\}$
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- Benefit: adapt to local variability.

Conformal prediction under covariate shift: weighted conformal inference [TFBCR19]

- New data may not i.i.d with previous data

$$(X_i, Y_i) \overset{\text{i.i.d.}}{\sim} P = P_X \times P_{Y|X}, i = 1, \ldots, n,$$

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- Construction: $C_{\text{split}}^w(x) = [\widehat{\mu}(x) - Q_{1-\alpha}^w, \widehat{\mu}(x) + Q_{1-\alpha}^w]$

$$\mathbb{P}\left(Y_{n+1} \in C_{\text{split}}^w(X_{n+1})\right) \geq 1 - \alpha$$

Inference of counterfactuals? Potential outcomes

Unit	X_i	T_i	$Y_i(1)$	$Y_i(0)$	Y_i^{obs}
Treatment Group					
1	✓	1	✓	x	$Y_1(1)$
2	✓	1	✓	x	$Y_2(1)$
3	✓	1	✓	x	$Y_3(1)$
4	✓	1	✓	x	$Y_4(1)$
5	✓	1	✓	x	$Y_5(1)$
Control Group					
6	✓	0	x	✓	$Y_6(0)$
7	✓	0	x	✓	$Y_7(0)$
8	✓	0	x	✓	$Y_8(0)$
9	✓	0	x	✓	$Y_9(0)$
10	✓	0	x	✓	$Y_{10}(0)$

Inference of counterfactuals? Potential outcomes [LC20]

Assumption

- stable unit treatment values (SUTVA)
- (i.i.d.)
- unconfoundedness $(Y(1), Y(0)) \perp\!\!\!\perp T \mid X$

- Individual treatment effect(ITE) τ_i is defined as

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- **Goal**: find interval estimate $\hat{C}_t(X)$, s.t.,

$$\mathbb{P}\left(Y(t) \in \hat{C}_t(X) \mid T = 1\right) \geq 1 - \alpha, \quad (t = 0, 1)$$

Counterfactual inference

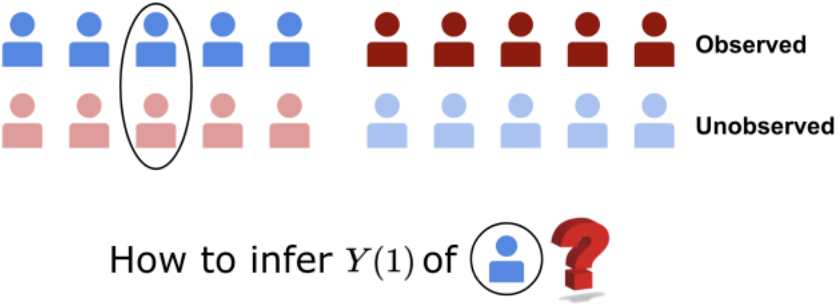
Assign treatment by a coin toss for each subject based on the propensity score e(x)

$$\mathbb{P}(\text{treated} \mid X = x) = e(x)$$

$$\mathbb{P}(\text{control} \mid X = x) = 1 - e(x)$$

Each subject has potential outcomes $(Y(1), Y(0))$ and the observed outcome Y^{obs}

Counterfactual inference



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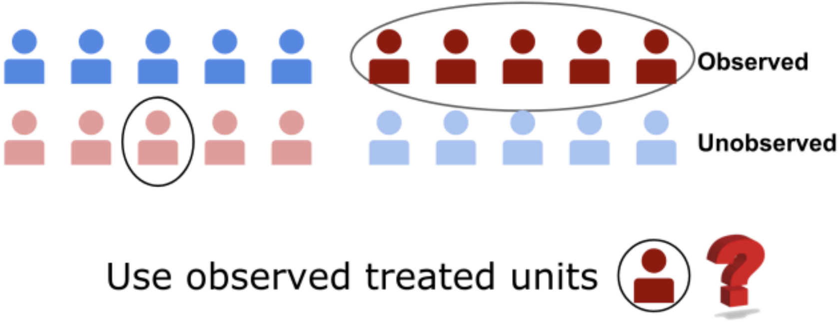
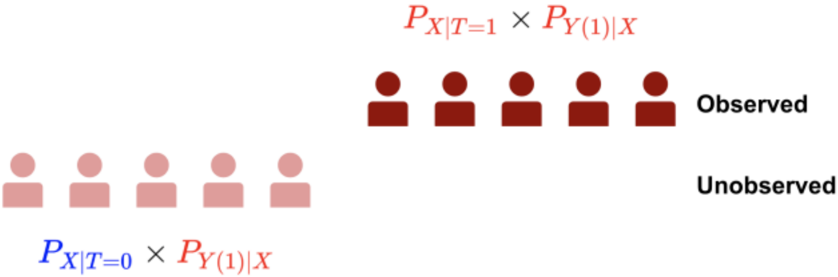


Covariate shift under unconfoundedness $Y(1) \perp\!\!\!\perp T \mid X$



Counterfactual inference

$$(X_i, Y_i^{\text{obs}}) \overset{i.i.d.}{\sim} P_{X|T=0} \times P_{Y(0)|X}$$

$$(X_i, Y_i^{\text{obs}}) \overset{i.i.d.}{\sim} P_{X|T=1} \times P_{Y(1)|X}$$

Use i.i.d. samples (observed treated units) from $P_{X|T=1} \times P_{Y(1)|X}$ to construct $\hat{C}_1(X)$ with

$$\mathbb{P}\Big(Y(1) \in \hat{C}_1(X)\Big) \geq 90\% \text{ under } P_{X|T=0} \times P_{Y(1)|X}$$

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Bad even if we have oracle quantile $\tilde{q}_\alpha(X)$, $q_\alpha(x)$

$$\mathbb{P}\left(T \geq q_\alpha(x) \mid X = x\right) = 1 - \alpha = \mathbb{P}\left(\widetilde{T} \geq \tilde{q}_\alpha(x) \mid X = x\right)$$

$$= \mathbb{P}\left(T \geq \tilde{q}_\alpha(x) \mid X = x\right) \mathbb{P}\left(C \geq \tilde{q}_\alpha(x) \mid X = x\right)$$

Survival data

- Observations: $\{(X_i, \tilde{T}_i, \Delta_i)\}_{i=1}^n$ i.i.d.
- Event indicator $\Delta_i = I(T_i < C_i)$:

$$\tilde{T}_i = \begin{cases} T_i & \text{if } \Delta_i = 1 \\ C_i & \text{if } \Delta_i = 0 \end{cases} \Rightarrow \tilde{T}_i = \min(T_i, C_i)$$

- Conditional independent censoring: $T \perp\!\!\!\perp C \mid X$
- Objective:

$$\mathbb{P}(T_{n+1} \geq \hat{L}(X_{n+1})) \geq 1 - \alpha$$

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Treat T as a "potential outcome" under the "treatment" $\Delta = 1$?

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- Invalid because "unconfoundedness" does not hold:

$$(T, C) \not\perp I(T < C) \mid X$$

$(X_i, T_i)_{\Delta_i = 1}$ has shifts in both the covariate distribution and conditional distribution

- What group should we condition on?

Leveraging the censoring mechanism[CLR23]

- Small censoring time is bad → condition on group with larger censoring time? E.g. $C \geq c_0$
- Obviously $(X, C, T) \overset{d}{\neq} (X, C, T) \mid C \geq c_0$.

$$P_{(X,\widetilde{T})|C\geq c_0} = P_{X|C\geq c_0} \times P_{\widetilde{T}|X,C\geq c_0}$$

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- We can build a lower bound for $T_{n+1} \wedge c_0$ via weighted conformal

$$\frac{dP_X}{dP_{X|C\geq c_0}}(x) = \frac{\mathbb{P}(C \geq c_0)}{\mathbb{P}(C \geq c_0 \mid X = x)}$$

The essence of conformal method

- Non-conformity score(S): how well a sample Z conforms to rest of data, if S is large, we say that Z is non-conforming or ”strange”.

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  - H_0: X_{n+1} follow same distribution with observed data[BCL+21]
  - H_0: Two-sample conditional distribution are equal [HL23]

Testing for outliers with conformal p-value [BCL+21]

$$\mathcal{D} = \mathcal{D}^{\text{train}} \cup \mathcal{D}^{\text{cal}}, \quad |\mathcal{D}^{\text{train}}| = |\mathcal{D}^{\text{cal}}| = n$$

- Clean i.i.d observed data from P_X, given many testing data want to test $\mathcal{H}_{0,i} : X_i \sim P_X$, for any $X_i \in \mathcal{D}^{\text{test}}$

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$$\hat{u}^{(\text{marg})}(X_i) = \frac{1 + \left|\left\{j \in \mathcal{D}^{\text{cal}} : \hat{s}\left(X_j\right) \leq \hat{s}(X_i)\right\}\right|}{n+1}$$

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End of presentation

All models are wrong, but some are (hopefully) useful

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All models are wrong, but **conformal** can make them safe and useful!

Thanks!

Reference I

- Stephen Bates, Emmanuel Candès, Lihua Lei, Yaniv Romano, and Matteo Sesia, Testing for outliers with conformal p-values, arXiv preprint arXiv:2104.08279 (2021).
- Emmanuel Candès, Lihua Lei, and Zhimei Ren, Conformalized survival analysis, Journal of the Royal Statistical Society Series B: Statistical Methodology **85** (2023), no. 1, 24–45.
- Xiaoyu Hu and Jing Lei, A two-sample conditional distribution test using conformal prediction and weighted rank sum, Journal of the American Statistical Association (2023), 1–19.
- Lihua Lei and Emmanuel J Candès, Conformal inference of counterfactuals and individual treatment effects, arXiv preprint arXiv:2006.06138 (2020).

Reference II

- Jing Lei, Max GSell, Alessandro Rinaldo, Ryan J Tibshirani, and Larry Wasserman, Distribution-free predictive inference for regression, Journal of the American Statistical Association **113** (2018), no. 523, 1094–1111.
- Yaniv Romano, Evan Patterson, and Emmanuel Candes, Conformalized quantile regression, Advances in neural information processing systems **32** (2019).
- Ryan J Tibshirani, Rina Foygel Barber, Emmanuel Candes, and Aaditya Ramdas, Conformal prediction under covariate shift, Advances in neural information processing systems **32** (2019).