Localized Conformal Prediction

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1 Conformal Prediction General[1]

Definition 1.1 (Exchangeability). *[3] For any r.v. $x_1, \cdots, x_k$, we say they are exchangeable if for any permutation $\sigma : [k] \to [k]$(bijection), $(x_1, \cdots, x_k) \stackrel{d.}{=} (x_{\sigma(1)}, \cdots, x_{\sigma(k)})$.*

Definition 1.2 (Weighted Exchangeability). *[4] For any r.v. $x_1, \cdots, x_k$, we say they are weighted exchangeable if their joint density canbe factorized as*

$$f(x_1, \cdots, x_k) = \prod_{i=1}^{k} w_i(x_i) \cdot g(x_1, \cdots, x_k),$$

where g is exchangeable, i.e., $g(x_1, \cdots, x_k) = g(x_{\sigma(1)}, \cdots, x_{\sigma(k)})$.

For conformal prediction two classes of targets are studied.

Definition 1.3 (Marginal Coverage). *$(X, Y) \in \mathbb{R}^p \times \mathbb{R} \sim P_{XY}$ which is unknown. Given training set $Tr = \{(X_i, Y_i)\}_{i=1}^n$, and test on (X_{n+1}, Y_{n+1}), both i.i.d.*

C_α satisfies distribution-free marginal coverage at level $1 - \alpha$ if

$$P(Y_{n+1} \in C_\alpha(X_{n+1})) \geq 1 - \alpha, \ \forall P_{XY}$$

The probability is with respect to $\{(X_i, Y_i)\}_{i=1}^{n+1}$.

Definition 1.4 (Conditional Coverage). *$(X, Y) \in \mathbb{R}^p \times \mathbb{R} \sim P_{XY}$ which is unknown. Given training set $Tr = \{(X_i, Y_i)\}_{i=1}^n$, and test on (X_{n+1}, Y_{n+1}), both i.i.d.*

C_α *satisfies distribution-free marginal coverage at level* $1-\alpha$ *if*

$$P\left(Y_{n+1} \in C_\alpha(X_{n+1}) \middle| X_{n+1} = x\right) \geq 1-\alpha,\ \forall P_{XY}$$

The probability is with respect to $\{(X_i, Y_i)\}_{i=1}^n$ *and* Y_{n+1}.

Definition 1.5 (Conformal Score Function)**.** *For data pair* (X, Y) *and point predictor and any loss function* $V(\cdot,\cdot)$*, call* $R = S(X,Y) = V(Y, \hat{f}(X))$ *be the conformal score(or residual).*

Definition 1.6 (Efficiency)**.** X *is some r.v. following the testing distribution and* C_α *is efficient if* $\mathbb{E}\left[|C_\alpha(X)|\right]$ *is small. Define Size*$(C_\alpha) = \frac{1}{n}\sum_{i=1}^{n}|C_\alpha(X_i)|$.

2 Localized CP Article1

Conformalized Quantile Regression [2]

The core idea is if conditional distribution function $F(y|X=x)$ is known and conditional quantile is $q_\alpha(x) = \inf\{y : F(y|X=x) \geq \alpha\}$, for $\alpha_1 = \alpha/2,\ \alpha_2 = 1-\alpha/2$ we can define conformal set to be $C_\alpha(x) = [q_{\alpha_1}(x), q_{\alpha_2}(x)]$. Next is to estimate quantiles from data.

Follow the split CP setting,

- First divide training set D into two sets: D_1 for proper training set and D_2 for calibration set. And let $n_i = |D_i|$, fit point predictor $\hat{q}_{\alpha_1},\ \hat{q}_{\alpha_2}$ on D_1.
- Calculate cnformity scores on calibration set: $R_i = \max\{\hat{q}_{\alpha_1}(X_i) - Y_i, Y_i - \hat{q}_{\alpha_2}(X_i)\}$ for $i \in D_2$, and $R = \max\{\hat{q}_{\alpha_1}(X) - Y_i, Y_i - \hat{q}_{\alpha_2}(X)\}$
- Find the $\lceil (1-\alpha)(n_2+1) \rceil$-th empirical quantile of $R_i,\ i \in D_2$ as $\hat{q}$ and construct conformal set $C_\alpha(x) = [\hat{q}_{\alpha_1}(x) - \hat{q}, \hat{q}_{\alpha_2}(x) + \hat{q}]$

Note that $\{Y \in C_\alpha(X)\} = \{R \leq \hat{q}\}$. With exchangeability of $R_i,\ i \in D_2$ and R the coverage is assured.

References

[1] Anastasios N Angelopoulos, Stephen Bates, et al. Conformal prediction: A gentle introduction. *Foundations and Trends® in Machine Learning*, 16(4):494–591, 2023.

[2] Yaniv Romano, Evan Patterson, and Emmanuel Candes. Conformalized quantile regression. *Advances in neural information processing systems*, 32, 2019.

[3] Glenn Shafer and Vladimir Vovk. A tutorial on conformal prediction. *Journal of Machine Learning Research*, 9(3), 2008.

[4] Ryan J Tibshirani, Rina Foygel Barber, Emmanuel Candes, and Aaditya Ramdas. Conformal prediction under covariate shift. *Advances in neural information processing systems*, 32, 2019.