Federated Conformal Prediction General

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May 17, 2024

1 Conformal Prediction General[1]

Definition 1.1 (Exchangeability). *[6] 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). *[7] 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 (Conditional Validity)**.** *[8] Call a conformal set C_α is (ε, δ) valid if*

$$P(\{X : P(Y \in C_\alpha(X)) \geq 1-\varepsilon\}) \geq 1-\delta,$$

which means we have enough, probability $1-\delta$, X makes conditional coverage is guaranteed.

Definition 1.6 (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 1.7 (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 Standard Split Conformal Prediction

- 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 $\hat{f}_1$ on D_1.
- Calculate residuals on D_2: $R_i = \left|Y_i - \hat{f}_1(X_i)\right|,\ i \in D_2$.
- Find quantile on calibration residuals: $\hat{q}_2 = \lceil(1-\alpha)n_2\rceil$ smallest of $R_i,\ i \in D_2$.
- Construct a conformal set: $C_\alpha(x) = \left[\hat{f}_1(x) - \hat{q}_2, \hat{f}_1(x) + \hat{q}_2\right]$.

Let $R_{n+1} = \left|Y_{n+1} - \hat{f}_1(X_{n+1})\right|$. Let rank statistic $R_{(j)}$ be the j-th smallest in $R_i,\ i \in D_2$, and $k_\alpha = \lceil(1-\alpha)(n_2+1)\rceil$. As

$$\{Y_{n+1} \in C_\alpha(X_{n+1})\} = \{R_{n+1} \leq \hat{q}_2\} = \left\{R_{n+1} \leq R_{(k_\alpha)}\right\},$$

and $R_i,\ i \in D_2,\ R_{n+1}$ are exchangeable, we have

$$\mathbb{P}\left(Y_{n+1} \in C_\alpha(X_{n+1}) \middle| D_1\right) \in \left[1-\alpha, 1-\alpha+\frac{1}{n_2+1}\right).$$

Assume a more general score function $V(x, y) = V((x, y); \hat{f}_1)$, define $R_i = V(X_i, Y_i)$ and change the conformal set to

$$C_\alpha(x) = \left\{y : S(x, y) = V(y, f(x)) \leq R_{(k_\alpha)}\right\}.$$

Remark 2.1. *Further condition on calibration set, which means conditioning on entire training set D and assume $R = V(x, y)$ has distribution F. As*

$$\{Y_{n+1} \in C_\alpha(X_{n+1})\} = \left\{R_{n+1} \leq R_{(k_\alpha)}\right\},$$

Assume the distribution function of $R_{(j)}$ is $F_{(j)}$, and we have

$$\begin{aligned}
\mathbb{P}\left(\mathbb{P}\left(Y_{n+1} \in C_\alpha(X_{n+1})\Big|D\right) \leq t\right) &= \mathbb{P}\left(\mathbb{P}\left(R_{n+1} \leq R_{(k_\alpha)}\Big|D\right) \leq t\right) \\
\text{condition on } D \text{ randomness comes from } R_{n+1}, &= \mathbb{P}\left(F(R_{(k_\alpha)}) \leq t\right) \\
&= \mathbb{P}\left(R_{(k_\alpha)} \leq F^{-1}(t)\right) \\
&= F_{(k_\alpha)}(F^{-1}(t)) \qquad (1)
\end{aligned}$$

rank statistic has density $F'_{(j)}(x) = jC^j_{n_2}x^{j-1}(1-x)^{n-j}f(x)$, thus take derivative on formula (1), and $\mathbb{P}\left(Y_{n+1} \in C_\alpha(X_{n+1})\Big|D\right)$ has density

$$k_\alpha C^{k_\alpha}_{n_2} t^{k_\alpha - 1}(1-t)^{n-k_\alpha}.$$

3 Standard Full Conformal Prediction

Full CP has similar steps as split CP. It uses all data points for training.

- Fix any x and trial data y to construct training set $\{(X_1, Y_1), \cdots, (X_n, Y_n), (x, y)\}$.
- Train point predictor $\hat{f}$ on training set and define residuals $R_i = \left|Y_i - \hat{f}(X_i)\right|,\ i \in [n],\ R_{n+1} = \left|y - \hat{f}(x)\right|$.
- Define j-th rank statistic of $R_i,\ i \in [n]$ as $R_{(j)}$, $k_\alpha = \lceil(1-\alpha)(n_2+1)\rceil$, and conformal set
$$C_\alpha(x) = \left\{y : R_{n+1} \leq R_{(k_\alpha)}\right\}.$$

As $\{Y_{n+1} \in C_\alpha(X_{n+1})\} = \left\{R_{n+1} \leq R_{(k_\alpha)}\right\}$, and the exchangebility of data

$$\mathbb{P}\left(Y_{n+1} \in C_\alpha(X_{n+1})\right) \in \left[1-\alpha, 1-\alpha+\frac{1}{n+1}\right).$$

4 Standard CP under covariate shift

Follow the procedure of split CP and heterogeneity between training and test data[7]. Assume

$$Z_i = (X_i, Y_i) \sim P = P_X \times P_{Y|X}, i = 1, \cdots, n,$$

$$Z_{n+1} = (X_{n+1}, Y_{n+1}) \sim P' = P'_X \times P_{Y|X}.$$

- Fix any trial data y to construct training set $\{(X_1, Y_1), \cdots, (X_n, Y_n), (X_{n+1}, y)\}$. Train point predictor $\hat{f}$ on new training set.

- Calculate nonconformity scores $R_i = S(X_i, Y_i),\ i \in \{1, \cdots, n\},\ R_{n+1} = S(X_{n+1}, y)$ based on $\hat{f}$.

- Calculate importance weights p_i based on likelihood ratio w:

$$w(x) = \frac{dP'_X(x)}{dP_X(x)},$$

$$p_i = \frac{w(X_i)}{\sum\limits_{j=1}^{n+1} w(X_j)},\ i = 1, \cdots, n+1.$$

- Calculate $1-\alpha$ quantile of distribution $\sum\limits_{i=1}^{n} p_i \delta_{R_i} + p_{n+1}\delta_\infty$ as q_α. Define conformal set $C_\alpha(x) = \{y : R_{n+1} \le q_\alpha\}$.

All independent variables are weighted exchangeable. Let E_Z be $\{Z_1, \cdots, Z_{n+1}\} = \{z_1, \cdots, z_{n+1}\}$. Assume joint density is $f(z_1, \cdots, z_{n+1}) = \prod\limits_{i=1}^{n+1} dP(z_i) \cdot w(x_{n+1})$. Condition on E_Z, calculate R_i based on $\hat{f}$ and z_i, for all permutation σ

$$\mathbb{P}\left(R_{n+1} = r_i \middle| E_Z\right) = \mathbb{P}\left(Z_{n+1} = z_i \middle| E_Z\right) = \frac{\sum\limits_{\sigma(n+1)=i} f\big(z_{\sigma(1)}, \cdots, z_{\sigma(n+1)}\big)}{\sum\limits_{\sigma} f\big(z_{\sigma(1)}, \cdots, z_{\sigma(n+1)}\big)} = p_i,$$

which leads to $R_{n+1}\Big|E_Z \sim \sum\limits_{i=1}^{n+1} p_i \delta_{r_i}$. Let $Q(1-\alpha, F)$ be the quantile function,

$$\mathbb{P}\left(R_{n+1} \le Q(1-\alpha, \sum_{i=1}^{n+1} p_i \delta_{r_i}) \middle| E_Z\right) \ge 1 - \alpha,$$

means

$$\mathbb{P}\left(R_{n+1} \leq Q(1-\alpha, \sum_{i=1}^{n} p_i \delta_{r_i} + p_{n+1}\delta_\infty) \Big| E_Z\right) \geq 1-\alpha,$$

as condition on E_Z, $\sum\limits_{i=1}^{n} p_i \delta_{r_i} + p_{n+1}\delta_\infty = \sum\limits_{i=1}^{n} p_i \delta_{R_i} + p_{n+1}\delta_\infty$(left p is based on z and right based on Z). The p_i in following formula is different from previous one.

$$\mathbb{P}\left(R_{n+1} \leq Q(1-\alpha, \sum_{i=1}^{n} p_i \delta_{R_i} + p_{n+1}\delta_\infty) \Big| E_Z\right) \geq 1-\alpha,$$

thus taking expectation on all E_Z,

$$\mathbb{P}\left(Y_{n+1} \in C_\alpha(X_{n+1})\right) = \mathbb{P}\left(R_{n+1} \leq q_\alpha\right) \geq 1-\alpha$$

5 Standard CP under Nonexchangeability

Conformal Prediction Beyond Exchangeability[2]

When data is not exchangeable, like covariate shift setting, standard CP is not valid. This article gives a more general method under unknown distribution nonexchangeability.

Definition 5.1 (Total Variation of Distribution). *Given two distribution with density $p(x)$, $q(x)$ the total variation is defined as*

$$d_{TV}(p,q) = \frac{1}{2}\int |p(x)-q(x)|dx$$

Assume data $Z = \{(Z_1 = (X_1, Y_1), t_1), \cdots, (Z_{n+1} = (X_{n+1}, Y_{n+1}), t_{n+1})\}$ and Z^k be data sequence swap Z_k and Z_{n+1} in Z(t remains the same), $Z^{n+1} = Z$. Train a asymmetric point estimator based on Z^k call $\hat{f}^k$. And let the residual of sample i based on $\hat{f}^k$ be $R_i^k = |Y_i - \hat{f}^k(X_i)|$. Given weights $w_i,\ i = 1, \cdots, n+1$ and choose $K = i$ with probability w_i. Define conformal set

$$C_\alpha(X_{n+1}) = \left\{ y : R_{n+1}^K \leq Q(1-\alpha, \sum_{i=1}^{n+1} w_i \delta_{R_i^K}) \right\}.$$

First calculate

$$\begin{aligned}
\{Y_{n+1} \notin C_\alpha(X_{n+1})\} &= \left\{ R_{n+1}^K > Q(1-\alpha, \sum_{i=1}^{n+1} w_i \delta_{R_i^K}) \right\} \\
&= \left\{ R_{n+1}^K > Q(1-\alpha, \sum_{i=1}^{n} w_i \delta_{R_i^K} + w_{n+1}\delta_\infty) \right\}
\end{aligned}$$

notice

$$
\begin{aligned}
\sum_{i=1}^{n} w_i \delta_{R_i^K} + w_{n+1}\delta_\infty &= \sum_{i\neq K} w_i \delta_{R_i^K} + w_K(\delta_{R_K^K} + \delta_\infty) + (w_{n+1} - w_K)\delta_\infty \\
\text{As } \delta_\infty \leq \delta_x, \forall x \in \mathbb{R}, \ &\leq \sum_{i\neq K} w_i \delta_{R_i^K} + w_K(\delta_{R_K^K} + \delta_{R_{n+1}^K}) + (w_{n+1} - w_K)\delta_\infty \\
\text{As } w_{n+1} \geq w_K, \ &\leq \sum_{i\neq K} w_i \delta_{R_i^K} + w_K(\delta_{R_K^K} + \delta_{R_{n+1}^K}) + (w_{n+1} - w_K)\delta_{R_K^K} \\
&= \sum_{i\neq K} w_i \delta_{R_i^K} + w_K \delta_{R_{n+1}^K} + w_{n+1}\delta_{R_K^K},
\end{aligned}
$$

thus

$$
Q(1-\alpha, \sum_{i=1}^{n} w_i \delta_{R_i^K} + w_{n+1}\delta_\infty) \geq Q(1-\alpha, \sum_{i\neq K} w_i \delta_{R_i^K} + w_K \delta_{R_{n+1}^K} + w_{n+1}\delta_{R_K^K}),
$$

and

$$
\{Y_{n+1} \notin C_\alpha(X_{n+1})\} \subset \left\{ R_{n+1}^K \geq Q(1-\alpha, \sum_{i\neq K} w_i \delta_{R_i^K} + w_K \delta_{R_{n+1}^K} + w_{n+1}\delta_{R_K^K}) \right\}.
$$

Let $R^k = (R_1^k, \cdots, R_{k-1}^k, R_{n+1}^k, R_{k+1}^k, \cdots, R_n^k, R_k^k)$, $r = (r_1, \cdots, r_{n+1})$ and $S(r) = \{j \in [n+1] : r_j > Q(1-\alpha, \sum_{i=1}^{n+1} w_i \delta_{r_i})\}$. As assume $r = R^k$, $r_k = R_{n+1}^k$

$$
\left\{ R_{n+1}^K \geq Q(1-\alpha, \sum_{i\neq K} w_i \delta_{R_i^K} + w_K \delta_{R_{n+1}^K} + w_{n+1}\delta_{R_K^K}) \right\} = \left\{ K \in S(R^K) \right\}.
$$

Finally we have

$$
\begin{aligned}
P(\{Y_{n+1} \notin C_\alpha(X_{n+1})\}) &\leq P(K \in S(R^K)) \\
&= \sum_{i=1}^{n+1} w_i P(i \in S(R^i)),
\end{aligned}
$$

notice

$$
P(i \in S(R^i)) = \int_{\Omega_i} dP(R^i) \leq \int_{\Omega_i} dP(R^{n+1}) + \int \left| dP(R^i) - dP(R^{n+1}) \right|,
$$

thus

$$
\begin{aligned}
P(\{Y_{n+1} \notin C_\alpha(X_{n+1})\}) &\leq P(K \in S(R^K)) \\
&= \sum_{i=1}^{n+1} w_i P(i \in S(R^{n+1})) + \sum_{i=1}^{n} w_i d_{TV}(R^i, R^{n+1}).
\end{aligned}
$$

6 Federated Conformal Prediction Article1

Efficient Conformal Prediction under Data Heterogeneity[5]

Idea: The marginal coverage is measured over all training data and test points. However, if there is a high variability in the coverage probability as a function of the training data, the test coverage probability may be substantially below $1-\alpha$ for a particular training set.

Definition 6.1 (empirical miscoverage rate)**.** $\alpha(Tr) = P(Y_{n+1} \notin C_\alpha(X_{n+1})|Tr)$

In this article, assume n agents each has calibration data $(X_k^i, Y_k^i) \sim P_X^i P_{Y|X},\ k = 1, \cdots, n^i,\ i = 1, \cdots, n$, and calibration set $D_i = \{(X_k^i, Y_k^i)\}_{k=1}^{n_i},\ i = 1, \cdots, n$. Let calibration distribution be $P^{cal} = \sum\limits_{i=1}^{n} \pi_i P_X^i P_{Y|X}$, where $\pi_i = n_i / \left(\sum\limits_{j=1}^{n} n_j\right)$, and the test distribution $P^{test} = P_X^{n+1} P_{Y|X}$. Let the general density ratio be $w(x,y) = \frac{dP_X^{n+1}(x)}{\sum\limits_{i=1}^{n} \pi_i dP_X^i(x)}$.

- Utilize the GMM to compute parameters $\{\pi_y^i, \mu_y^i, \Sigma_y^i\}_{y \in \mathcal{Y}^i}$ on D_i. Note that P_X^i is approximated by $|\mathcal{Y}^i|$ centers mixed GMM, $P_X^i = \sum\limits_{y \in \mathcal{Y}^i} \pi_y^i N(\phi(x); \mu_y^i, \Sigma_y^i),\ i = 1, \cdots, n+1$, where $\phi()$ be some latent map used while training $\hat{f}$. Further $w(x,y)$ can be calculated.

- Fix any trial data y, similar to covariate shift setting, a common idea should be calculate importance weight $p_k^i = w(X_k^i, Y_k^i)/W,\ k = 1, \cdots, n^i,\ i = 1, \cdots, n$, where $W = \sum\limits_{i=1}^{n} \sum\limits_{k=1}^{n^i} w(X_k^i, Y_k^i) + w(X_{n+1}, y)$, and $p_{n+1} = w(X_{n+1}, y)/W$. Similarly define residuals $R_k^i,\ R_{n+1}$.

- Conformal set: $C_\alpha(X_{n+1}) = \left\{ y : R_{n+1} \le Q(1-\alpha, \sum\limits_{i=1}^{n} \sum\limits_{k=1}^{n^i} p_k^i \delta_{R_k^i} + p_{n+1}\delta_\infty) \right\}$.

7 Federated Conformal Prediction Article2

Federated Conformal Predictors for Distributed Uncertainty Quantification[4]

The federated learning setting is similar to article1, but specific with classification setting. Data $(X_k^i, Y_k^i) \sim P^i,\ k = 1, \cdots, n_i,\ i = 1, \cdots, n$ be calibration distribution for each i-th agent. The test distribution is $P^{test} = \sum_{i=1}^{n} \lambda_i P^i$. And $X \in \mathcal{X},\ Y \in \mathcal{Y}$, where $\mathcal{Y}$ has finite items.

Definition 7.1 (FL Exchangeability)**.** *Follow previous setting and* $(X,Y) \sim P^{test}$. *The scores on i-th agent* $S(X_1^i, Y_1^i), \cdots, S(X_{n_i}^i, Y_{n_i}^i), S(X,Y)$ *are exchangeable with probability* λ_i.

Remark 7.2. *FL exchangebility means the test distribution is the mixture of all agent distribution and with probability* λ_i, (X,Y) *has distribution* P^i.

- Write $N = \sum_{i=1}^{n} n_i$, $\lambda_i = (n_i+1)/(N+n)$.
- Fix trial data y for new test X. Calculate scores on each agent with given global classifier f, $\{R_k^i = S(X_k^i, Y_k^i)\}_{i\in[n], k\in[n_i]}$ and $R = S(X,y)$.
- Define conformal set $C_\alpha(X) = \{y : R \le \hat{q}_\alpha\}$, where $\hat{q}_\alpha$ is the $\lceil (1-\alpha)(N+n) \rceil$ smallest of agent scores.

Let $n_i(q) = |\{k \le n_i : R_k^i \le q\}|$ and $\sum_{i=1}^{n} n_i(\hat{q}_\alpha) = \lceil (1-\alpha)(N+n) \rceil$. Define event

$$E = \left\{ \forall i \in [n],\ \{R_k^i\}_{k=1}^{n_i} = \{r_k^i\}_{k=1}^{n_i} \right\}.$$

Then first follow FL exchangebility the whole space can be divided into n disjoint subspace $\Omega_i = \{R_1^i, \cdots, R_{n_i}^i, R \text{ are exchangeable}\}$. And (X,Y) belongs to which P^i is independent of all other things.

$$P(R \le \hat{q}_\alpha \Big| E) = \sum_{i=1}^{n} \lambda_i P(R \le \hat{q}_\alpha \Big| E, \Omega_i).$$

Similar to results in split CP, $P(R \le \hat{q}_\alpha \Big| E, \Omega_i) \ge n_i(\hat{q}_\alpha)/(n_i+1)$ as $n_i(\hat{q}_\alpha)$ scores are smaller than $\hat{q}_\alpha$ in $R_1^i, \cdots, R_{n_i}^i$ which are exchangeable with R. Thus,

$$P(R \le \hat{q}_\alpha \Big| E) \ge \sum_{i=1}^{n} \lambda_i \frac{n_i(\hat{q}_\alpha)}{n_i+1} = \frac{\sum_{i=1}^{n} n_i(\hat{q}_\alpha)}{N+n} = \frac{\lceil (1-\alpha)(N+n) \rceil}{N+n} \ge 1-\alpha.$$

8 Federated Conformal Prediction Article3

One-Shot Federated Conformal Prediction[3]

Still assume a similar setting, data $(X_k^i, Y_k^i) \sim P^i,\ k = 1, \cdots, m,\ i = 1, \cdots, n$ be calibration distribution for each i-th agent. And scores $R^i = (R_1^i, \cdots, R_m^i)$ for i-th agent.

Core idea of this article is: if each agent gives a quantile $\hat{q}_\alpha^i$, further find a quantile of these quantiles to generate the conformal set.

- Each agent compute scores R^i, given α calculate k' , l'
- Each agent returns k'-th smallest score to the central server $R^i_{(k')}$
- Central server find l'-th smallest of $\{R^i_{(k')}\}_{i=1}^n$ $\hat{q}$. Define conformal set $C_\alpha(X) = \{y : R = S(X, y) \leq \hat{q}\}$

The decision of $k',\ l'$ is easy to understand.

$$\{Y \in C_\alpha(X)\} = \{R \leq R^{(l')}_{(k')}\},$$

where $R^{(l')}_{(k')}$ is the l'-th smallest of $R^i_{(k')}$. Order statistic has explicit distribution, assume $R^i_k \sim G$, then $R^i_{(k)} \sim \sum\limits_{j=k}^{m} C_m^j G^j (1 - G)^{m-j}$, and further calculate the quantile of quantile can get the distribution of $\hat{q}$. This implies $k',\ l'$ can be find through simple calculation.

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