

Chap. 4: Conditional Coverage

Sunghee Park

Dept. of Statistics
Seoul National University

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Conditional Coverage of the Conformal Prediction

- We have already guaranteed the marginal coverage of the conformal prediction.

$$1 - \alpha \leq \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}))$$

- This chapter focuses on the conditional coverage, which is $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1})|W)$ and satisfies the equation below:

$$\mathbb{E}[\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1})|W)] = \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}))$$

- However, that relationship doesn't guarantee

$$1 - \alpha \leq \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1})) \Rightarrow 1 - \alpha \leq \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1})|W)$$

AT ALL.

What this chapter will cover

Recall that the conditional coverage is $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1})|W)$.

This chapter will cover

- Training-conditional coverage (W is related to \mathcal{D})
- Test-conditional coverage (W is related to X_{n+1})
- and others...

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Goals and Assumptions

The goal is to make $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | \mathcal{D}) > 1 - \alpha$ almost surely.

For some theoretical support of the conditional coverage, we need to make strong assumptions.

- We assume split conformal prediction. Which means that the score $s((x, y); \mathcal{D})$ and \mathcal{D} are independent.
- The data points are i.i.d

If then, we can conclude Theorem 4.1 below.

Theorem 4.1. Distribution of the training conditional coverage

With previous assumptions,

$$\begin{aligned} \mathbb{P}(\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | \mathcal{D}_n) \leq 1 - \alpha - \Delta) \\ \leq F_{\text{Beta}((1-\alpha)(n+1), \alpha(n+1))}(1 - \alpha - \Delta) \leq e^{-2n\Delta^2}, \end{aligned}$$

Sketch of the proof of Theorem 4.1

- Let $s(X, Y) \sim F$ (CDF), $(X, Y) \sim P$, $S_i \sim F$ (i.i.d)
- By the algorithm of the CP, we can induce that

$$Y_{n+1} \in \mathcal{C}(X_{n+1}) \Leftrightarrow S_{n+1} \leq S_{(k)} \quad (k = \lceil (1 - \alpha)(n + 1) \rceil)$$

and

$$\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid \mathcal{D}_n) = \mathbb{P}(S_{n+1} \leq S_{(k)} \mid \mathcal{D}_n) = F(S_{(k)})$$

- Since $S_i \sim F$, by using the basic property of CDF (sim. as Probability integral transform), $F(S_i) \sim U_i$ and F preserves the order, (monotone increase) $F(S_{(i)}) \sim U_{(i)}$,
Let $U_i \sim U[0, 1]$ (i.i.d)

$$\begin{aligned} & \mathbb{P}(F(S_{(k)}) \leq 1 - \alpha - \Delta) = \mathbb{P}(U_{(k)} \leq 1 - \alpha - \Delta) \\ & \leq \mathbb{P}(U_{(k)}^* \leq 1 - \alpha - \Delta) = F_{\text{Beta}((1-\alpha)(n+1), \alpha(n+1))}(1 - \alpha - \Delta) \end{aligned}$$

holds since the property of Beta distribution.

The meaning of Theorem 4.1

Theorem 4.1. Distribution of the training conditional coverage

With previous assumptions,

$$\begin{aligned} \mathbb{P}(\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid \mathcal{D}_n) \leq 1 - \alpha - \Delta) \\ \leq F_{\text{Beta}((1-\alpha)(n+1), \alpha(n+1))}(1 - \alpha - \Delta) \leq e^{-2n\Delta^2}, \end{aligned}$$

- This theorem implies when we choose α' for CP, which is 'stricter' than α , we can make

$$\mathbb{P}(\mathbb{P}(Y_{n+1} \notin \mathcal{C}(X_{n+1}) \mid \mathcal{D}_n) \leq \alpha) \geq 1 - \delta$$

- In detail, we can choose α' as:

$$F_{\text{Beta}((1-\alpha')(n+1), \alpha'(n+1))}(1 - \alpha) = \delta$$

- It no longer guarantee in only the 'exchangeable' data (c.f. marginal case)

Since the beta-dist. was from iid of $(X, y) \rightarrow \{S_i\} \rightarrow \{U_i\}$

Hardness result for training-conditional coverage

Actually, it is impossible to fully guarantee training conditional coverage for full conformal prediction

Theorem 4.3. Hardness result for training-conditional coverage

Let P be any distribution on $\mathcal{X} \times \mathcal{Y}$ s.t. $P_{\mathcal{X}}$ is nonatomic*, there exists symmetric conformal score ftn s s.t. when running full conformal prediction with this choice of s ,

$$\mathbb{P}(\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | \mathcal{D}_n) = 0) \geq \alpha - O\left(\sqrt{\frac{\log n}{n}}\right)$$

where the probability is taken with respect to the training set $\mathcal{D}_n = ((X_1, Y_1), \dots, (X_n, Y_n))$ drawn i.i.d. from P .

*nonatomic $\Leftrightarrow \text{atom}(P) = \{z | \mathbb{P}_P(z) > 0\} = \emptyset$

Sketch of the proof of Theorem 4.3

- Constructive Proof
- Since P is nonatomic, $\exists a : \mathcal{X} \rightarrow \{0, 1, \dots, n-1\}$ with $a(X)$ has a equal prob. in domain when $X \sim P$
- For dataset $\mathcal{D} = ((x_1, y_1), \dots, (x_k, y_k))$ and an additional data point (x, y) , Consider

$$s((x, y); \mathcal{D}) = \mathbb{1} \left\{ \text{mod} \left(-a(x) + \sum_{j=1}^k a(x_j), n \right) < N \right\}$$

- This score has quite useful properties in the proof:
 - Its domain is $\{0, 1\}$ - Simply think coverage fail only
 $S_{n+1} = 1 \wedge \hat{q} = 0 \Rightarrow \alpha_P(\mathcal{D}_n) = \mathbb{P}(S_{n+1} = 1, \hat{q} = 0 | \mathcal{D}_n)$
 - $S_{n+1} = s((X_{n+1}, Y_{n+1}); \mathcal{D}_{n+1}) =$
 $\mathbb{1} \{ \text{mod} (\sum_{i=1}^n a(X_i), n) < N \}$ (ftn unrelated to test point)
- Define \mathcal{E}_{mod} as the event that $\text{mod} (\sum_{i=1}^n a(X_i), n) < N$.

Sketch of the proof of Theorem 4.3 (Cont')

- Let $\alpha_P(\mathcal{D}_n) := \mathbb{P}(Y_{n+1} \notin \mathcal{C}(X_{n+1}) \mid \mathcal{D}_n) = \mathbb{1}_{\mathcal{E}_{\text{mod}}} \cdot \mathbb{P}(\text{Quantile}(S_1, \dots, S_{n+1}; 1 - \alpha) = 0 \mid \mathcal{D}_n)$
- Using Sliding Window Method : Let $W_k = \{i \in \{0, \dots, n-1\} : \text{mod}(-i + k - 1, n) \geq N\}$, let $\mathcal{E}_{\text{unif}}$ be the event that

$$\sum_{i=1}^n \mathbb{1}\{a(X_i) \in W_k\} \geq (1 - \alpha)(n + 1) \text{ for all integers } k,$$

i.e., each window of indices W_k contains a sufficient fraction of the sample.

- $S_i = \mathbb{1}\{a(X_i) \notin W_{1+\sum_j a(X_j)}\}$ and by the property of $\mathcal{E}_{\text{unif}}$.

$$\mathbb{P}(\alpha_P(\mathcal{D}_n) = 1) \geq \mathbb{P}(\mathcal{E}_{\text{mod}} \cap \mathcal{E}_{\text{unif}}) \geq \mathbb{P}(\mathcal{E}_{\text{mod}}) - \mathbb{P}(\mathcal{E}_{\text{unif}}^c) = \frac{N}{n} - \mathbb{P}(\mathcal{E}_{\text{unif}}^c)$$

- Make upper bound of $\mathbb{P}(\mathcal{E}_{\text{mod}})$ using tail-prob. of Binomial dist. and set $N = \alpha n - O(n \log n)$

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Goals

The goal is to make $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | X_{n+1}) > 1 - \alpha$ almost surely.

CP satisfying conditional coverage on discrete X

CP satisfying conditional coverage on discrete X

- Suppose that $\mathcal{X} = \{x_1, x_2, \dots, x_{|\mathcal{X}|}\}$ then
 $\mathcal{C}(x_k) = \{y : s(x_k, y) \leq \hat{q}_k\}$ where
 $\hat{q}_k = \text{Quantile}((S_i)_{i \in [n], X_i = x_k}; (1 - \alpha)(1 + 1/n_k))$
- Similar to the naive CP, but now, we choose the quantile in a smaller group which has same X value.
- This will make the similar result to the naive CP when the dist. of $s(X, Y)|X = x_i$ are similar.
- The detailed proof will be discussed later.

CP satisfying conditional coverage on continuous X

- Actually, there is no "nice" prediction method which satisfying the conditional coverage on continuous X almost surely.

Theorem 4.4.

Suppose \mathcal{C} is any procedure that satisfies distribution-free conditional coverage, i.e., for any distribution P on $\mathcal{X} \times \mathcal{Y}$, $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid X_{n+1}) \geq 1 - \alpha$ holds almost surely, where the probability is taken with respect to

$(X_1, Y_1), \dots, (X_{n+1}, Y_{n+1}) \stackrel{\text{i.i.d.}}{\sim} P$.

Then, for any distribution P on $\mathcal{X} \times \mathcal{Y}$ for which the marginal P_X is nonatomic, $\mathbb{P}(y \in \mathcal{C}(x)) \geq 1 - \alpha$ for every $(x, y) \in \mathcal{X} \times \mathcal{Y}$

Sketch of the proof of Theorem 4.4

- For all $(x, y) \in \mathcal{X} \times \mathcal{Y}$ and $\epsilon > 0$
- Using "Distridution-Free" feature of \mathcal{C} , Define a mixture dist.

$$P' = (1 - \epsilon)P + \epsilon\delta_{(x,y)}$$
- Since $\mathbb{P}_{P'}(X_{n+1} = x) > 0$, by assumption,

$$\mathbb{P}_{P'}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid X_{n+1} = x) \geq 1 - \alpha$$
- Moreover, P_X is nonatomic from the assumption,

$$\mathbb{P}_{P'}(Y_{n+1} = y \mid X_{n+1} = x) = 1$$
 and

$$\mathbb{P}_{P'}(y \in \mathcal{C}(X_{n+1}) \mid X_{n+1} = x) = \mathbb{P}_{P'}(y \in \mathcal{C}(x)) \geq 1 - \alpha$$
- We can conclude

$$\mathbb{P}_P(y \in \mathcal{C}(x)) \geq \mathbb{P}_{P'}(y \in \mathcal{C}(x)) - d_{TV}(P^n, P'^n) \geq 1 - \alpha - n\epsilon$$

CP satisfying conditional coverage on continuous X

(Cont.)

Corollary 4.5. Lebesgue measure limitations of the continuous case.

Suppose \mathcal{C} is any procedure that satisfies distribution-free conditional coverage, i.e., for any distribution P on $\mathcal{X} \times \mathcal{Y}$,

$$\mathbb{P}(\text{Leb}(\mathcal{C}(x)) = \infty) \geq 1 - \alpha$$

where $\text{Leb}(\cdot)$ denotes the Lebesgue measure.

Proof of Corollary 4.5.

- By definition of Lebesgue measure,

$$\begin{aligned}\text{Leb}(\mathcal{C}(x)) &= \int_{\mathbb{R}} \mathbb{1}\{y \in \mathcal{C}(x)\} dy \leq a \implies \int_{y=0}^{a+b} \mathbb{1}\{y \in \mathcal{C}(x)\} dy \leq a \\ &\iff \int_{y=0}^{a+b} \mathbb{1}\{y \notin \mathcal{C}(x)\} dy \geq b.\end{aligned}$$

- Apply Markov's Inequality and Fubini's thm,

$$\begin{aligned}\mathbb{P}(\text{Leb}(\mathcal{C}(x)) \leq a) &\leq \mathbb{P}\left(\int_{y=0}^{a+b} \mathbb{1}\{y \notin \mathcal{C}(x)\} dy \geq b\right) \\ &\leq \frac{\mathbb{E}\left[\int_{y=0}^{a+b} \mathbb{1}\{y \notin \mathcal{C}(x)\} dy\right]}{b} = \frac{\int_{y=0}^{a+b} \mathbb{P}(y \notin \mathcal{C}(x)) dy}{b} \leq \frac{(a+b)\alpha}{b}\end{aligned}$$

- Take $b \rightarrow \infty$ and $a \rightarrow \infty$ in order

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Relaxation Approach on test-conditional coverage

- So far, we concluded that it is impossible to achieve pointwise test-conditional coverage in continuous setting.
- One of the idea is relaxing the problem to discrete version - which is easily available.
- New goal: $1 - \alpha \leq \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | \mathcal{X}_k)$ for $k \in [K]$ with $P(\mathcal{X}_k) > 0$

CP satisfying new goal (Binned Conditional Coverage)

- $\mathcal{C}(X_{n+1}) = \{y : s(X_{n+1}, y) \leq q_k(\hat{x}_{n+1})\}$ where $\hat{q}_k = \text{Quantile}((S_i)_{i \in [n], X_i \in \mathcal{X}_k}; (1 - \alpha)(1 + 1/n_k))$
- Similar to the naive CP, but now, we choose group-(score) quantile \mathcal{X}_i

Label-conditional coverage

- Goal : to make $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | Y_{n+1}) > 1 - \alpha$ almost surely

CP satisfying the goal (Label-conditional coverage)

- $\mathcal{C}(X_{n+1}) = \{y : S_{n+1}^y \leq \hat{q}^y\}$ where
 $\hat{q}^y = \text{Quantile}((S_i)_{i \in \mathcal{I}_y}; (1 - \alpha)(1 + 1/|\mathcal{I}_y|))$, $\mathcal{I}_y = \{i \in [n] : Y_i = y\}$
- Similar to the naive CP, but now, we group by y

Mondrian CP : Generalized CP

- Binned Conditional Coverage ($g(x, y) = k$ ($x \in \mathcal{X}_k$)) and Label-conditional coverage ($g(x, y) = y$) are the special cases.
- General Goals : to make

$$\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) | g(X_{n+1}, Y_{n+1})) \geq 1 - \alpha \text{ w.p.1}$$

Mondrian Conformal Prediction

- $\mathcal{C}(X_{n+1}) = \{y : S_{n+1}^y \leq \hat{q}^y\}$ where

$$\hat{q}^y = \text{Quantile} \left((S_i)_{i \in \mathcal{I}_{g(X_{n+1}, y)}}; (1 - \alpha)(1 + 1/|\mathcal{I}_{g(X_{n+1}, y)}|) \right),$$

$$\mathcal{I}_k = \{i \in [n] : g(X_i, Y_i) = k\}$$
- CP with 'Grouping'

Proof of the validity of Mondrian CP

- First, we should show the statement below holds.

Lemma 4.7. Conditional exchangeability within a bin

Suppose $(X_1, Y_1), \dots, (X_{n+1}, Y_{n+1})$ are exchangeable. Fix any subset $\mathcal{Z}_0 \subseteq \mathcal{X} \times \mathcal{Y}$, and for any fixed nonempty subset $I \subseteq [n+1]$, let \mathcal{E}_I be the event that $\{i \in [n+1] : (X_i, Y_i) \in \mathcal{Z}_0\} = I$. If \mathcal{E}_I has positive probability, then $((X_i, Y_i))_{i \in I}$ is exchangeable conditional on \mathcal{E}_I .

- The key of the proof is that for arbitrary $\sigma \in \text{perm}(I)$, think the extended permutation $\tilde{\sigma} \in \text{perm}([n+1])$ which satisfies the following equation and apply the exchangeability in $[n+1]$ wisely to show $\mathbb{P}((Z_i)_{i \in I} \in A, \mathcal{E}_I) = \mathbb{P}((Z_{\sigma(i)})_{i \in I} \in A, \mathcal{E}_I)$

$$\tilde{\sigma}(i) = \begin{cases} \sigma(i) & i \in I \\ i & i \notin I \end{cases}$$

Proof of the validity of Mondrian CP (Cont')

- Then, we prove the main theorem.
- First, by construction of the set $\mathcal{C}(X_{n+1})$, we can see that for any $k \in [K]$, on the event $g(X_{n+1}, Y_{n+1}) = k$,

$$Y_{n+1} \in \mathcal{C}(X_{n+1}) \iff \bar{p} := \frac{1 + \sum_{i \in [n], g(X_i, Y_i) = k} \mathbb{1}\{S_i \geq S_{n+1}\}}{1 + |\mathcal{I}_k|} > \alpha$$

- Next, fix any label $k \in [K]$ with $\mathbb{P}(g(X_{n+1}, Y_{n+1}) = k) > 0$, and let $\mathcal{Z}_0 = \{(x, y) \in \mathcal{X} \times \mathcal{Y} : g(x, y) = k\} \subseteq \mathcal{X} \times \mathcal{Y}$. By Lemma, the quantity

$$p = \frac{1 + \sum_{i \in [n]} \mathbb{1}\{(X_i, Y_i) \in \mathcal{Z}_0, S_i \geq S_{n+1}\}}{1 + \sum_{i \in [n]} \mathbb{1}\{(X_i, Y_i) \in \mathcal{Z}_0\}} = \bar{p}$$

satisfies $\mathbb{P}(p \leq \alpha \mid g(X_{n+1}, Y_{n+1}) = k) \leq \alpha$.

This completes the proof.

Another Relaxation on test-conditional coverage

- Another idea relaxing the problem is to weaken the condition of X .
- New goal: $\mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid X_{n+1} \in \mathcal{X}_0) \geq 1 - \alpha$ for all P , and all $\mathcal{X}_0 \subseteq \mathcal{X}$ with $P_X(\mathcal{X}_0) \geq \delta$.
- Trivial Solution : much more strict target "Marginal coverage level" and use randomization

CP satisfying new goal

- 1 Construct $\mathcal{C}'(X_{n+1})$, using any method that guarantees marginal coverage at level $1 - c\alpha\delta$.
- 2 With probability $\frac{1-\alpha}{1-c\alpha}$, return $\mathcal{C}(X_{n+1}) = \mathcal{C}'(X_{n+1})$; otherwise, return $\mathcal{C}(X_{n+1}) = \emptyset$.

Prove of the previous method

- By construction of the method, we have

$$\begin{aligned} & \mathbb{P}(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid X_{n+1} \in \mathcal{X}_0) \\ &= \frac{1 - \alpha}{1 - c\alpha} \mathbb{P}(Y_{n+1} \in \mathcal{C}'(X_{n+1}) \mid X_{n+1} \in \mathcal{X}_0) \end{aligned}$$

- Next

$$\begin{aligned} & \mathbb{P}(Y_{n+1} \notin \mathcal{C}'(X_{n+1}) \mid X_{n+1} \in \mathcal{X}_0) \\ & \leq \delta^{-1} \mathbb{P}(Y_{n+1} \notin \mathcal{C}'(X_{n+1})) \mathbb{1}_{X_{n+1} \in \mathcal{X}_0} \leq \delta^{-1} \cdot c\alpha\delta = c\alpha \end{aligned}$$

Combining these two calculations proves the result.

Lower bound of the CI length in prev. method

Definition : L_P

let $L_P(1 - t)$ be the minimum length of any *oracle* prediction interval \mathcal{C}_{1-t}^P which is constructed given knowledge of the distribution P (i.e., not a distribution-free method), and has coverage level $1 - t$:

$$L_P(1 - t) = \inf \{ \mathbb{E}_P[\text{Leb}(\mathcal{C}_{1-t}^P(X))] : \mathcal{C}_{1-t}^P \text{ satisfies } \mathbb{P}_P(Y \in \mathcal{C}_{1-t}^P(X)) \geq 1 - t \}.$$

Theorem 4.13. Lower Bound of CI-length of the \mathcal{C}

Suppose \mathcal{C} satisfies the distribution-free relaxed test-conditional coverage condition, and let $\mathcal{Y} = \mathbb{R}$. Then, for any distribution P on $\mathcal{X} \times \mathbb{R}$ for which the marginal P_X is nonatomic,

$$\mathbb{E}[\text{Leb}(\mathcal{C}(X_{n+1}))] \geq \inf_{c \in [0,1]} \left\{ \frac{1 - \alpha}{1 - c\alpha} \cdot L_P(1 - c\alpha\delta) \right\}.$$

Lower bound of the CI length in prev. method (Cont.)

- to prove the previous theorem, we need some lemmas.

Lemma 4.14

Suppose \mathcal{C} satisfies the distribution-free relaxed test-conditional coverage condition. Let P be any distribution on $\mathcal{X} \times \mathcal{Y}$ s.t the marginal P_X is nonatomic, then

$$\mathbb{P}_P(Y_{n+1} \in \mathcal{C}(X_{n+1}) \mid (X_{n+1}, Y_{n+1}) \in B) \geq 1 - \alpha$$

for any $B \subseteq \mathcal{X} \times \mathcal{Y}$ with $P(B) \geq \delta$

Lower bound of the CI length in prev. method (Cont.)

- to prove the previous theorem, we need some lemmas.

Lemma 4.15. The sample–resample construction

Let P be a distribution on \mathcal{Z} , and let $m, M \geq 1$. Let P^m denote the corresponding product distribution on \mathcal{Z}^m —that is, the distribution of (Z_1, \dots, Z_m) , where $Z_1, \dots, Z_m \stackrel{\text{i.i.d.}}{\sim} P$. Moreover, let Q denote the distribution on \mathcal{Z}^m obtained by the following process to generate (Z_1, \dots, Z_m) :

- 1 Sample $Z^{(1)}, \dots, Z^{(M)} \stackrel{\text{i.i.d.}}{\sim} P$, and define the empirical distribution $\hat{P}_M = \frac{1}{M} \sum_{i=1}^M \delta_{Z^{(i)}}$;
- 2 Sample $Z_1, \dots, Z_m \stackrel{\text{i.i.d.}}{\sim} \hat{P}_M$.

Then

$$d_{\text{TV}}(P^m, Q) \leq \frac{m(m-1)}{2M},$$

where d_{TV} denotes the total variation distance between distributions.

Thank you!

References I

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