An introduction to conformal prediction sets

Draft notes of E. ROQUAIN

disclaimers: • not exhaustive (very active area)
• prediction sets for response ≠ confidence region for parameter

Classical review paper: [Angelopoulos and Bates (2022)] is very nice historical notes on Vovk

Road map:

I Setting

1. Notation and aim
2. Non-conformity score function

II Classical methods

1. Naive method
2. Split conformal method
3. Full conformal method
4. Cross-validated conformal method

III Some extensions

1. Nested prediction sets
2. Conditional guarantees
3. Beyond exchangeability
4. Transductive approach

I Setting

(1) Notation and aim

- Let (X_i, Y_i) random variables with
  - X_i: covariate
  - Y_i: outcome

  $X_i \in \mathbb{R}^d$ d possibly large (for simplicity, it could be image, graph, ...)

  $Y_i \in \mathcal{Y}$ e.g. $\mathcal{Y} = \{1, \dots, K\}$ classification or $\mathcal{Y} = \mathbb{R}$ regression

- (X_i, Y_i) are iid $\sim P$ (unknown) over several samples:

  $\mathcal{D} = ((X_1, Y_1), \dots, (X_n, Y_n))$ full training sample observed

  $\mathcal{D}_{test} = (X_{n+1}, Y_{n+1})$ test sample
  - X_{n+1}: observed
  - Y_{n+1}: not observed

Aim: build $\hat{\mathcal{C}}_\alpha(\cdot; \mathcal{D}) \subset \mathcal{Y}$ such that

$$\mathbb{P}\left(Y_{n+1} \in \hat{\mathcal{C}}_\alpha(X_{n+1}; \mathcal{D})\right) \geq 1 - \alpha$$

"prediction set"

⊕ true for any distribution P (or weak assumption like no ties)

⊕ true for any sample size $n \geq 1$

⊕ can be combined with any "machine learning" algorithm

⊖ $\hat{\mathcal{C}}_\alpha = \mathcal{Y}$ allowed (not necessarily informative)

(2) Non-conformity score function

Measurable function $S(\cdot; D) : (x, y) \in \mathbb{R}^d \times \mathcal{Y} \mapsto \mathbb{R}$

- regression $S(x, y; D) = |y - \hat{\mu}(x, D)|$ "residual"

  for $\hat{\mu}(x, D)$ estimator of $\mu(x) = \mathbb{E}[Y_1 \mid X_1 = x]$

- classification $S(x, y; D) = 1 - \hat{\pi}_x(y; D)$ "proba that label y is not predicted in x"

  for $\hat{\pi}_x(y; D)$ estimator of $\pi_x(y) = \mathbb{P}(Y_1 = y \mid X_1 = x)$

$S(x, y; D)$ is large if y does not conform to the prediction in x

II Classical methods

(1) Naive method

- Compute $S_i = S(X_i, Y_i; D)$, $1 \le i \le n$

  ↳ empirical distribution of 'typical' non conformity scores

- Take q_α "some quantile" of this distribution

- Choose $\hat{C}_\alpha(X_{n+1}, D) = \{y \in \mathcal{Y} : S(X_{n+1}, y; D) \le q_\alpha\}$

  as prediction set

⚠ fail in general : under interpolation $S_i = 0$, $1 \le i \le n$ ⚠

↳ only works asymptotically, with a good predictor !

The problem is that D is used both for prediction and for evaluating the quality of the prediction

② Split conformal method

[Papadopoulos et al. (2002)] = inductive = split conformal

Split D into

$$D_{train} = ((X_i, Y_i),\ i \in I_{train}) \quad \text{size } n_{train}$$
$$D_{cal} = ((X_i, Y_i),\ i \in I_{cal}) \quad \text{size } n_{cal}$$

- Non-conformity score function $S(x, y; D_{train})$
- Scores $S_i = S(X_i, Y_i; D_{train})$, $i \in I_{cal}$
- Take $q_\alpha = (1-\alpha)$-quantile of $(S_i, i \in I_{cal}) \cup \{+\infty\}$

$$= (1-\alpha)\left(1+\frac{1}{n_{cal}}\right)\text{-quantile of } (S_i, i \in I_{cal})$$
$$= S_{(\lceil (1-\alpha)(n_{cal}+1) \rceil)}$$

for $S_{(1)} \leq \dots \leq S_{(n_{cal})} \leq S_{(n_{cal}+1)} = +\infty$

Then the split conformal prediction set is given by

$$\hat{C}_\alpha^{split}(X_{n+1}, D) = \{y \in \mathcal{Y} : S(X_{n+1}, y; D_{train}) \leq q_\alpha\}$$

Examples :

* **regression** : prediction interval

$\hat{\mu}(x, D_{train})$ estimator of $\mu(x) = \mathbb{E}[Y_1 \mid X_1 = x]$ can be anything ! (OLS, NN, RF, ...)

$S_i = |Y_i - \hat{\mu}(X_i, D_{train})|$, $i \in I_{cal}$

split

$$\hat{C}_\alpha(X_{n+1}, D) = \{y \in \mathcal{Y} : |y - \hat{\mu}(X_{n+1}, D_{train})| \leq q_\alpha\}$$

$$= \left[\hat{\mu}(X_{n+1}, D_{train}) - q_\alpha, \hat{\mu}(X_{n+1}, D_{train}) + q_\alpha\right]$$

Illustration good predictor $\Leftrightarrow$ q_α small $\Leftrightarrow$ small interval

* **classification** : prediction label set

$\hat{\pi}_x(y; D_{train})$ estimator of $\pi_x(y) = \mathbb{P}(Y_1 = y \mid X_1 = x)$ (RNN, NN, ...)

$S_i = 1 - \hat{\pi}_{X_i}(Y_i; D_{train})$, $i \in I_{cal}$

split

$$\hat{C}_\alpha(X_{n+1}, D) = \{y \in \mathcal{Y} : 1 - \hat{\pi}_{X_{n+1}}(y; D_{train}) \leq q_\alpha\}$$

$$= \{y \in \mathcal{Y} : \hat{\pi}_{X_{n+1}}(y; D_{train}) \geq 1 - q_\alpha\}$$

Note that the threshold $1 - q_\alpha$ is not $1 - \alpha$

↳ on garde les labels $y \in \mathcal{Y}$ les plus probables au vu des scores de références.

good classification $\Leftrightarrow$ q_α small $\Leftrightarrow$ few labels in $\hat{C}_\alpha$

Proposition : $\forall P, \forall (n_{train}, n_{cal})$,

$$\mathbb{P}\left(Y_{n+1} \in \hat{\mathcal{C}}^{split}_{\alpha}(X_{n+1}; \mathcal{D}_{train})\right) \geq 1-\alpha$$

and if $\mathbb{P}(S_i = S_j) = 0 \quad \forall i \neq j$ $\quad \leq 1 - \alpha + \frac{1}{n_{cal}+1}$

split conformal is valid with accuracy $\simeq \frac{1}{n_{cal}}$

Proof : $S_{n+1} = S(X_{n+1}, Y_{n+1}; \mathcal{D}_{train})$

- $Y_{n+1} \notin \hat{\mathcal{C}}_{\alpha}(X_{n+1}; \mathcal{D}_{train}) \Leftrightarrow S_{(n_\alpha)} < S_{n+1}$, $n_\alpha = \lceil (1-\alpha)(n_{cal}+1) \rceil$

$$\Leftrightarrow \sum_{i \in I_{cal}} \mathbb{1}\{S_i < S_{n+1}\} \geq n_\alpha$$

$$\Leftrightarrow \sum_{i \in I_{cal} \cup \{n+1\}} \mathbb{1}\{S_i < S_{n+1}\} \geq (1-\alpha)(n_{cal}+1)$$

$n_{cal}+1$ elements in $I_{cal} \cup \{n+1\}$

$$\Leftrightarrow \sum_{i \in I_{cal} \cup \{n+1\}} \mathbb{1}\{S_i \geq S_{n+1}\} \leq \alpha(n_{cal}+1)$$

$= \text{rank of } S_{n+1} \text{ in } \{S_1, \dots, S_{n_{cal}}, S_{n+1}\}$

- But $(X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$ iid

$\Rightarrow S_1, \dots, S_{n_{cal}}, S_{n+1}$ exchangeable $| \mathcal{D}_{train}$

if $S_i \neq S_j$ for $i \neq j$ almost surely then rank $\sim \mathcal{U}(1, \dots, n_{cal}+1)$

and $\mathbb{P}\left(Y_{n+1} \notin \hat{\mathcal{C}}_{\alpha}(X_{n+1}; \mathcal{D}_{train})\right) = \frac{\lceil \alpha(n_{cal}+1) \rceil}{n_{cal}+1}$ okay!

$\in \left[\alpha - \frac{1}{n_{cal}+1}, \alpha\right]$

in general, we have

Lemma [Romano and Wolf (2005)] (empirical p-values are super-uniform)

For $(Y_1, \dots, Y_B, Y_{B+1})$ any real valued exchangeable random vector

$$\mathbb{P}\left(\frac{1}{B+1} \sum_{b=1}^{B+1} \mathbb{1}\{Y_b \geq Y_{B+1}\} \leq \alpha \right) \leq \frac{[\alpha(B+1)]}{B+1} \leq \alpha$$

↳ $\geq \mathbb{P}$(score to $\geq$ observed score) 'empirical pvalue'

Proof: see for instance [Arlot et al. (2010)] proof Lemma 5.2

Here the empirical p value is: $\hat{p}(Y_{n+1}) = \frac{1}{n_{cal}+1} \sum_{i \in I_{cal} \cup \{n+1\}} \mathbb{1}\{S_i \geq S_{n+1}\}$

This shows $\mathbb{P}\left(Y_{n+1} \notin \hat{C}_\alpha(X_{n+1}; D_{train})\right) \leq \frac{[\alpha(n_{cal}+1)]}{n_{cal}+1} \leq \alpha$ □

Split conformal ⊕ easy to compute
⊖ splitting a bit arbitrary and sample waste

③ Full conformal method [Vovk et al (2005)]

Keep $D = ((X_1, Y_1), \dots, (X_n, Y_n))$ full training sample and train with $D \cup \{(X_{n+1}, Y_{n+1})\}$

- non conformity score function $S(x, y; D \cup \{(X_{n+1}, Y_{n+1})\})$ which is assumed permutation invariant w.r.t. sample
- scores $S_i(Y_{n+1}) = S(X_i, Y_i; D \cup \{(X_{n+1}, Y_{n+1})\})$, $1 \leq i \leq n+1$

$$\hat{C}_\alpha^{full}(X_{n+1}, D) = \left\{ y \in \mathcal{Y} : S_{n+1}(y) \leq S_{(\lceil (1-\alpha)(n+1) \rceil)}(y) \right\}$$

Proposition : $\forall P, \forall n,$

$$\mathbb{P}\left(Y_{n+1} \in \hat{C}^{\text{full}}_{\alpha}(X_{n+1}; \mathcal{D}_{\text{train}})\right) \geq 1-\alpha$$

and if $\mathbb{P}(S_i = S_j) = 0 \quad \forall i \neq j$ $\quad \leq 1-\alpha+\frac{1}{n+1}$

full conformal is valid

Proof by the previous proof, just have to show that

$(S_1, \dots, S_n, S_{n+1})$ are exchangeable

Clear because $\forall \sigma$ permutation of $\{1, \dots, n+1\}$

$$(S_{\sigma(i)},\ 1 \leq i \leq n+1) = (S(X_{\sigma(i)}, Y_{\sigma(i)}; ((X_j, Y_j), 1 \leq j \leq n+1), 1 \leq i \leq n+1)$$

$$= (S(X_{\sigma(i)}, Y_{\sigma(i)}; ((X_{\sigma(j)}, Y_{\sigma(j)}), 1 \leq j \leq n+1), 1 \leq i \leq n+1)$$

↑ permutation invariance of score function

$$\sim (S(X_i, Y_i; (X_j, Y_j), 1 \leq j \leq n+1), 1 \leq i \leq n+1)$$

↑ because $(X_1, Y_1) \dots (X_{n+1}, Y_{n+1})$ are exchangeable $\square$

Full conformal ⊕ no sample splitting and 'cleaner'
⊖ difficult to compute

Possible to 'conformalize' . Ridge [Nouretdinov et al. (2001)]
. LASSO [Lei (2017)]
↳ see also the works of Eugène Ndiaye (Apple Paris)

④ Cross-validated conformal method

[Barber et al (2021)] = Jackknife +

Aim: ⊕ computable
⊕ no sample splitting
but ... ⊖ Loss of a factor 2 in the coverage

- score function $S(x, y; D')$ permutation invariant in sample D'
- scores $S_i = S(X_i, Y_i; D_{-i})$, $1 \le i \le n$ 'leave one out' = 'jackknife'
  $D_{-i} = (X_1, Y_1), \dots, (X_{i-1}, Y_{i-1}), (X_{i+1}, Y_{i+1}), \dots, (X_n, Y_n)$
- $\hat{p}(Y_{n+1}) = \frac{1}{n+1}\left(1 + \sum_{i=1}^{n} \mathbb{1}\{S_i \ge S(X_{n+1}, Y_{n+1}; D_{-i})\}\right)$
- $\hat{C}^{CV}_{\alpha}(X_{n+1}; D) = \{y \in \mathcal{Y} : \hat{p}(y) > \alpha\}$

Theorem: $\forall P, \forall n$, $\mathbb{P}\left(Y_{n+1} \in \hat{C}^{CV}_{\alpha}(X_{n+1}, D)\right) \ge 1 - 2\alpha + \frac{1}{n+1}$
(such that $S(X_i, Y_i, D'_{i,j})$ has no ties (a.s., with proof notation)) $\ge 1 - 2\alpha$
CV conformal is valid up to a factor 2

Proof Key point:

Lemma: for any binary "antisymetric" matrix A $p \times p$ with null diagonal
($A_{ij} \in \{0, 1\}$, $A_{ij} = 1 - A_{ji}$, $A_{ii} = 0$)

$$S(A) = \left\{1 \le i \le p : \sum_{j=1}^{p} A_{ij} \ge p(1-\alpha)\right\}$$

(nb of lines with that many "1")

is of cardinal $\le 2\alpha p - 1$

Proof: $\forall i \in S(A)$, we have

$$1 + \sum_{j \in S(A) \setminus \{i\}} (1 - A_{ij}) = \sum_{j \in S(A)} (1 - A_{ij}) \leq \sum_{j=1}^{p} (1 - A_{ij}) = p - \sum_{j=1}^{p} A_{ij} \leq p\alpha$$

for any pair $(k,\ell) \subset S(A)$ with $k \neq \ell$ let $(i,j) \subset S(A)$ s.t. $\{i,j\} = \{k,\ell\}$ and $A_{ij} = 0$

This makes at most $|S(A)|(p\alpha - 1)$ choices for a pair of $S(A)$

Thus $|S(A)|(|S(A)| - 1)/2 \leq |S(A)|(p\alpha - 1)$ □

Then let $D' = D \cup \{(X_{n+1}, Y_{n+1})\}$

$\forall (i,j) \in \{1..n+1\}^2$, $D'_{-i,-j}$ the set D' with (X_i, Y_i) and (X_j, Y_j) have been removed

$$R_{ij} = S(X_i, Y_i; D'_{-i,-j}) \quad \text{"residual in } i \text{ with sample } -i-j\text{"}$$

$$A_{ij} = \mathbb{1}\{R_{ij} > R_{ji}\} \quad \text{"score better in } i \text{ than } j\text{"}$$

A $(n+1)\times(n+1)$ binary "anti-symmetric" matrix ↑ true from (*)

Also, by exchangeability of $(X_1, Y_1), \ldots, (X_{n+1}, Y_{n+1})$, we have

$$\forall i, \quad \{R_{ij} - R_{ji},\ 1 \leq j \leq n+1\} \overset{\pi : i \leftrightarrow n+1}{\sim} \{R_{n+1,\pi(j)} - R_{\pi(j),n+1},\ 1 \leq j \leq n+1\}$$

$$= \{R_{n+1,j} - R_{j,n+1},\ 1 \leq j \leq n+1\}$$

↑ not ordered set

Thus $\forall i$, $\sum_{j=1}^{n+1} A_{ij} \overset{(*)}{\sim} \sum_{j=1}^{n+1} A_{n+1,j}$

Hence

$$\mathbb{P}\left(Y_{n+1} \notin \hat{C}_\alpha^{CV}(X_{n+1}, D)\right) = \mathbb{P}\left(\sum_{j=1}^{n} \mathbb{1}\{\underbrace{S(X_j, Y_j; D'_{-n+1,-j})}_{= R_{j,n+1}} < S(X_{n+1}, Y_{n+1}; D'_{-n+1,-j})\} \geq (n+1)(1-\alpha)\right)$$

$$= \mathbb{P}\left(\sum_{j=1}^{n+1} A_{n+1,j} \geq (n+1)\alpha\right)$$

$R_{n+1,j}$

put $\mathbb{E}$ outside

$$\overset{(*)}{=} \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{P}\left(\sum_{j=1}^{n+1} A_{ij} \geq (n+1)\alpha\right) = \mathbb{E}\left[\frac{|S(A)|}{n+1}\right] \leq \frac{2\alpha(n+1) - 1}{n+1}$$

$i \in S(A)$ ↑ Lemma □

Examples regression $S(X_i, Y_i; D_{-i}) = |Y_i - \hat{\mu}(X_i; D_{-i})|$

$\hat{p} > \alpha$

$$\Leftrightarrow 1 + \sum_{i=1}^{n} \mathbb{1}\left\{ \hat{\mu}(X_{n+1}, D_{-i}) - S_i \leq Y_{n+1} \leq \hat{\mu}(X_{n+1}, D_{-i}) + S_i \right\} > (n+1)\alpha$$

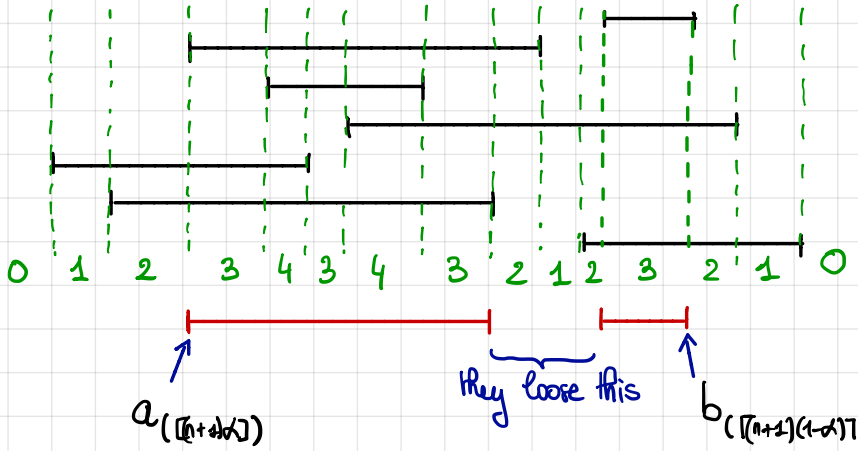
$(n \leq [x] \Leftrightarrow n \leq x)$

$$\Leftrightarrow \sum_{i=1}^{n} \mathbb{1}\left\{ \underbrace{\hat{\mu}(X_{n+1}, D_{-i}) - S_i}_{= a_i} \leq Y_{n+1} \leq \underbrace{\hat{\mu}(X_{n+1}, D_{-i}) + S_i}_{= b_i} \right\} \geq [(n+1)\alpha]$$

$$\Rightarrow \begin{cases} \sum_{i=1}^{n} \mathbb{1}\{ Y_{n+1} \leq b_i \} \geq [(n+1)\alpha] \\ \sum_{i=1}^{n} \mathbb{1}\{ a_i \leq Y_{n+1} \} \geq [(n+1)\alpha] \end{cases} \Leftrightarrow \begin{cases} Y_{n+1} \leq b_{([(n+1)(1-\alpha)])} \\ Y_{n+1} \geq a_{([(n+1)\alpha])} \end{cases}$$

[Barber et al (2021)] choose $\hat{C}_\alpha^{\text{jackknife+}} = \left[a_{([(n+1)\alpha])}, b_{([(n+1)(1-\alpha)])} \right]$

Illustration $(n+1)\alpha = 3$, $n = 7$, $[a_i, b_i]$, $1 \leq i \leq n$



classification : need to invert $\hat{\pi}_{X_{n+1}}(y; D_{-i})$ not explicit in general

III Some extensions

① Nested prediction sets [Gupta et al (2022)]

⚠ shape of prediction interval in regression very 'basic' ⚠

↳ $\hat{\mu}(x) \pm q_\alpha$

→ general approach encompassing many shapes of prediction sets

$\{\mathcal{F}_t(x; \mathcal{D}_{train})\}_{t \in \mathcal{T}}$ ⊂ y nested sequence of prediction sets

$\mathcal{T}$ ⊂ ℝ

nested: $\forall t \leq t'$, $\mathcal{F}_t(x; \mathcal{D}_{train}) \subseteq \mathcal{F}_{t'}(x; \mathcal{D}_{train})$

score function $S(x, y; \mathcal{D}_{train}) = \inf\{t \in \mathcal{T} : y \in \mathcal{F}_t(x; \mathcal{D}_{train})\}$

↳ smallest radius of the set capturing y

scores $S_i = S(X_i, Y_i; \mathcal{D}_{train})$ and usual split conformal (...)

→ also works with full / CV conformal (proofs for free!)

Reference	$\mathcal{F}_t(x)$	$\mathcal{T}$	Estimates
Lei et al. (2018)	$[\hat{\mu}(x) - t, \hat{\mu}(x) + t]$ usual	$[0, \infty)$	$\hat{\mu}$
Lei et al. (2018)	$[\hat{\mu}(x) - t\hat{\sigma}(x), \hat{\mu}(x) + t\hat{\sigma}(x)]$ locally weighted	$[0, \infty)$	$\hat{\mu}, \hat{\sigma}$
Romano et al. (2019)	$[\hat{q}_{\alpha/2}(x) - t, \hat{q}_{1-\alpha/2}(x) + t]$ conformalized quantile	$(-\infty, \infty)$	$\hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}$
Kivaranovic et al. (2019)	$(1+t)[\hat{q}_{\alpha/2}(x), \hat{q}_{1-\alpha/2}(x)] - t\hat{q}_{1/2}(x)$	$(-\infty, \infty)$	$\hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}, \hat{q}_{1/2}$
Sesia and Candès (2020)	$[\hat{q}_{\alpha/2}(x), \hat{q}_{1-\alpha/2}(x)] \pm t(\hat{q}_{1-\alpha/2}(x) - \hat{q}_{\alpha/2}(x))$	$(-1/2, \infty)$	$\hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}$
Chernozhukov et al. (2019)	$[\hat{q}_t(x), \hat{q}_{1-t}(x)]$	$(0, 1/2)$	$\{\hat{q}_\alpha\}_{\alpha \in [0,1]}$
Izbicki et al. (2019)	$\{y : \hat{f}(y\|x) \geqslant \check{t}_\delta(x)\}$[2]	$[0, 1]$	$\hat{f}$

② Conditional guarantees

→ conditional coverage is always more informative

* conditional on the full training sample $\mathcal{D}$

[Vovk (2012)], [Bian and Barber (2023)], [Liang and Barber (2023)]

Let $\alpha_P(\mathcal{D}) = \mathbb{P}\left(Y_{n+1} \notin \hat{C}_\alpha^{\text{split}}(X_{n+1}) \mid \mathcal{D}\right)$

Aim : $\mathbb{P}\left(\alpha_P(\mathcal{D}) \leq \alpha + \varepsilon\right) \geq 1-\delta$

Hoeffding : $\varepsilon = \sqrt{\frac{\log 1/\delta}{2 n_{\text{cal}}}}$ works (concentration of $S_{(\lceil (1-\alpha)(n_{\text{cal}}+1) \rceil)}$)

Is such result possible for full conformal/CV ?

- not for any predictor
- yes under a 'stability condition' for the predictor

* conditional on the new covariate X_{n+1}

Ideally, the prediction set should be tailored to the covariate X_{n+1}
↳ valid for all individuals with the same covariate X_{n+1}

$$\forall P, \forall n, \quad \mathbb{P}\left(Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \mid X_{n+1} = x\right) \overset{(*)}{\geq} 1-\alpha$$

for $P_{X_{n+1}}$-almost all x

[Vovk (2012)], [Lei and Wasserman (2014)]

Theorem : if (*) holds, and in the regression case, we have $\hat{C}_\alpha(\cdot)$ 'degenerated' :

$$\forall P, \quad \mathbb{P}_P\left(\left|\hat{C}_\alpha(x)\right| = \infty\right) \geq 1-\alpha \quad \text{for } P_{X_{n+1}} \text{ almost all } x \text{ not in the atoms of } P_{X_{n+1}}$$

Proof : if $\exists P$: $|\hat{C}_\alpha| < +\infty$ with proba $\geq \alpha$ build P' with $\forall$ Leye contradicting (*)

[Barber et al. (2020)] with a weaker aim only possible to say trivial things

Definition (conditional coverage)

$\hat{C}_{\alpha,S}$ does $(1-\alpha, S)$-CC, if

$$\mathbb{P}(Y_{n+1} \in \hat{C}_{\alpha,S}(X_{n+1}) \mid X_{n+1} \in \mathcal{X}) \geq 1-\alpha$$

for all P and $\mathcal{X} \subset \mathbb{R}^d$ with $P_X(\mathcal{X}) \geq S$

Theorem: $\forall \hat{C}_{\alpha,S}$ satisfying $(1-\alpha, S)$-CC, we have

$$\mathbb{E}[\Lambda(\hat{C}_{\alpha,S}(X_{n+1}))] \geq (1-\alpha) \inf_{\hat{C} \text{ with marginal cov} \geq 1-\alpha S} \mathbb{E}[\Lambda(\hat{C})]$$

↳ marginal cov at $1-\alpha S$ is essentially the best that you can do

↳ if (*) then $\mathbb{E}[\Lambda(\hat{C}_\alpha(X_{n+1}))] \geq \sup_S \{\dots\}$ large!

Definition (group conditional coverage)

$\hat{C}_\alpha$ such that $\mathbb{P}(Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \mid X_{n+1} \in G) \geq 1-\alpha$

for all P and $G \in \mathcal{G}$ (subsets of $\mathbb{R}^d$)

[Vovk et al. (2013)] Mondrian conformal prediction → non overlaping groups

[Jung et al. (2023)], [Gibbs et al. (2023)] More general solutions

* conditional on the new label Y_{n+1}

Investigated in classification → 'class specific coverage'

⚠ classical coverage provide more coverage for frequent classes ⚠

if $\mathcal{Y} = \{$Common Cold, Flu, Covid$\}$ maybe always predict $\hat{\mathcal{C}}_\alpha = \{$Common cold, Flu$\}$ has correct coverage

[Lei (2014)], [Sadinle et al. (2018)], [Derhacobian et al (202?)]

$$\forall P, \forall y \in \mathcal{Y}, \quad \mathbb{P}\left(Y_{n+1} \in \hat{\mathcal{C}}_\alpha(X_{n+1}) \mid Y_{n+1} = y \right) \geq 1 - \alpha$$

- all classes treated equally, so 'fair'
- kind of frequentist guarantee because unknown quantity y is fixed
  ≃ confidence region for the parameter y

Classical solution is to calibrate by separating the possible labels

③ Beyond exchangeability

* Covariate shift (= domain shift)

What if we calibrate with wrong data ? calibrate with 'dogs' evaluate on 'cats'

[Tibshirani et al. (2019)]

$$\begin{cases} (X_i, Y_i) \text{ iid } \sim P = P_X \times P_{Y|X} \\ (X_{n+1}, Y_{n+1}) \sim \tilde{P} = \tilde{P}_X \times P_{Y|X} \end{cases}$$

↙ covariate shift

Solution is to use weighted quantile / p-values with $w(x) = \frac{d\tilde{P}_X(x)}{dP_X(x)}$

↙ to compensate the covariate shift

Namely $\{Y_{n+1} \in \hat{C}_\alpha^{\text{wsplit}}(X_{n+1})\} = \{\hat{p}_\omega > \alpha\}$

with $S(X_i, Y_i; D_{\text{train}})$ — $S(X_{n+1}, Y_{n+1}; D_{\text{train}})$

$$\hat{p}_\omega = \frac{\omega(X_{n+1}) + \sum_{i \in I_{\text{cal}}} \omega(X_i) \mathbb{1}\{S_i \geq S_{n+1}\}}{\sum_{i \in I_{\text{cal}}} \omega(X_i) + \omega(X_{n+1})}$$

→ still provide coverage $1-\alpha$ (weighted exchangeability)

→ if weights unknown and estimated, remainder term [Jin and Candès (2023)]

* 'Almost' exchangeable case [Barber et al. (2023)]

- (X_i, Y_i)'s indep but $d_{TV}(\mathcal{L}(X_i, Y_i), \mathcal{L}(X_{n+1}, Y_{n+1}))$ not zero
- weights $\big|\ (\omega_i)_{i \in I_{\text{cal}}}$ fixed in $[0,1]^{n_{\text{cal}}}$, $\omega_{n+1} = 1$, $\tilde{\omega}_i = \frac{\omega_i}{\sum_{i \in I_{\text{cal}}} \omega_{i+1}}$ $i \in I_{\text{cal}} \cup \{n+1\}$
- weighted split conformal as above with

$$\hat{p}_\omega = \tilde{\omega}_{n+1} + \sum_{i \in I_{\text{cal}}} \tilde{\omega}_i \mathbb{1}\{S_i \geq S_{n+1}\}$$

weights to fight the d_{TV}

Theorem:

$$\mathbb{P}(Y_{n+1} \in \hat{C}_\alpha^{\text{wsplit}}(X_{n+1})) \geq 1 - \alpha - 2 \sum_{i=1}^{n} \tilde{\omega}_i \, d_{TV}(\mathcal{L}(X_i, Y_i), \mathcal{L}(X_{n+1}, Y_{n+1}))$$

↳ remainder

Example: $\begin{cases} d_{TV}(\mathcal{L}(X_i, Y_i), \mathcal{L}(X_{n+1}, Y_{n+1})) \leq \varepsilon\,(n+1-i) & \text{'time shift'} \\ \omega_i = \rho^{n+1-i} \end{cases}$

$\Rightarrow$ remainder $\leq 2\varepsilon \sum_{i=1}^{n} (n+1-i)\rho^{n+1-i} = 2\varepsilon \sum_{i=1}^{n} i\rho^i \leq \frac{2\varepsilon\rho}{(1-\rho)^2}$

④ Transductive approach [Vovk (2013)]

[Bates et al (2023)], [Marandon et al (2023)], [Gazin et al (2023)]

$\mathcal{D}_{test} = ((X_{n+1}, Y_{n+1}), \dots, (X_{n+m}, Y_{n+m}))$ test sample of size m

observed — not observed

Multiple prediction sets $(\hat{C}_{i,t})_{1 \le i \le m}$ such that

$$FCP(t) = \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}\{Y_{n+i} \notin \hat{C}_{i,t}\} \quad \text{is 'small' in probability}$$

$$= \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}\{\hat{p}_i \le t\} \quad \text{to study}$$

Split conformal: $\hat{p}_i = \frac{1}{n_{cal}+1} \left(1 + \sum_{j \in I_{cal}} \mathbb{1}\{S_j \ge S_{n+i}\}\right)$, $1 \le i \le m$

$(\hat{p}_i, 1 \le i \le m)$

- positive dependence [Bates et al (2023)]
- full distribution known
- concentration

} [Gazin et al (2023)] see also [Marques (2023)]

Theorem (DKW type concentration) Assume no ties in S_i's a.s.

$$\mathbb{P}\left(\sup_{t \in [0,1]} (FCP(t) - t) > \lambda\right) \le \left(1 + \frac{2\sqrt{2\pi\tau}}{\sqrt{n_{cal}+m}}\right) e^{-2\tau\lambda^2}$$

for $\tau := \frac{n_{cal} m}{n_{cal}+m} \in \left[\frac{1}{2} n_{cal} \wedge m, n_{cal} \wedge m\right]$ and $\lambda > 0$

$\Rightarrow$ with proba $\ge 1-\delta$, $\forall \alpha$, $FCP(\alpha) \le \alpha +$ remainder $\simeq \sqrt{\frac{\log \tau}{\tau}}$

References: (order of appearance)

[Angelopoulos and Bates (2022)] A gentle introduction to conformal prediction (...)

[Papadopoulos et al. (2002)] Inductive confidence machines for regression

[Romano and Wolf (2005)] Exact and approximate Stepdown methods for MT

[Arlot et al. (2010)] Some nonasympt results on resampling in high dim (I)

[Vovk et al. (2005)] Algorithmic learning in a random world

[Nouretdinov et al (2001)] Ridge regression confidence machine

[Lei (2017)] Fast exact conformalization of lasso using piecewise linear (...)

[Barber et al (2021)] Predictive inference with the jackknife+

[Gupta et al (2022)] Nested conformal prediction and quantile out of bags (...)

[Vovk (2012)] Conditional validity of inductive conformal predictor

[Bian and Barber (2023)] Training-conditional coverage for distribution free (...)

[Liang and Barber (2023)] Algo stability implies training-conditional coverage (...)

[Lei and Wasserman (2014)] Distribution free prediction bands for NP regression

[Barber et al. (2020)] The limits of distribution-free conditional predictive inf.

[Vovk et al. (2013)] Mondrian confidence machine

[Jung et al. (2023)] Batch multivalid conformal prediction

[Gibbs et al. (2023)] Conformal prediction with conditional guarantees

[Lei (2014)] Classification with confidence

[Sadinle et al. (2018)] Least ambiguous set-valued classifier with bounded error levels

[Derhacobian et al (202?)] Adaptive prediction sets with class cond. cov.

[Tibshirani et al.(2019)] Conformal prediction under covariate shift

[Jin and Candès (2023)] Model-free selective inf. under cov. shift via weighted conformal p-values

[Barber et al. (2023)] Conformal prediction beyond exchangeability

[Vovk (2013)] Transductive conformal predictor

[Bates et al (2023)] Testing for outliers with conformal p-values

[Marandon et al(2023)] Adaptive novelty detection with FDR guarantees

[Gazin et al (2023)] Transductive conformal inference with adaptive scores

[Kuchibhotla (2023)] On the universal distribution of the coverage in split conformal prediction