# Conformal prediction and its extensions

# 1 CP: Conformal prediction

Methods for distribution-free prediction.

### Assumption: exchangeability

- The data  $Z_i = (X_i, Y_i)$  are assumed to be exchangeable (for example, i.i.d.).
  - Definition (Vovk, Gammerman, and Shafer 2005; Shafer and Vovk 2008). Suppose that for any collection of N values, the N! different orderings are equally likely. Then we say that  $Z_1, \ldots, Z_N$  are exchangeable. The exchangeability assumption is slightly weaker than the i.i.d. assumption.
- The algorithm which maps data to a fitted model  $\hat{\mu}: \mathcal{X} \to \mathbb{R}$  is assumed to treat the data points symmetrically.
  - For example, OLS versus WLS.

#### 1.1 Split conformal prediction

(inductive conformal prediction)

- 1. initial training data set: pre-trained model  $\hat{\mu}: \mathcal{X} \to \mathbb{R}$ .
- 2. holdout/calibration set: nonconformity scores  $R_{i}=\left|Y_{i}-\hat{\mu}\left(X_{i}\right)\right|, \quad i=1,\ldots,n.$
- $\begin{aligned} &3. \text{ prediction set: } \widehat{C}_n\left(X_{n+1}\right) = \widehat{\mu}\left(X_{n+1}\right) \pm \mathbf{Q}_{1-\alpha}\left(\sum_{i=1}^n \frac{1}{n+1} \cdot \delta_{R_i} + \frac{1}{n+1} \cdot \delta_{+\infty}\right). \\ &\left(\text{the } \lceil (n+1)(1-\alpha) \rceil \text{th smallest of } R_1, \dots, R_n\right) \end{aligned}$

Drawback: the loss of accuracy due to sample splitting.

## 1.2 Full conformal prediction

(transductive conformal prediction)

1. training data & a hypothesized test point:  $\hat{\mu}^{y}=\mathcal{A}\left(\left(X_{1},Y_{1}\right),\ldots,\left(X_{n},Y_{n}\right),\left(X_{n+1},y\right)\right)$  for

 $\begin{aligned} &2. \text{ residuals: } R_{i}^{y} = \begin{cases} \left| Y_{i} - \hat{\mu}^{y}\left(X_{i}\right) \right|, & i = 1, \dots, n \\ \left| y - \hat{\mu}^{y}\left(X_{n+1}\right) \right|, & i = n+1 \end{cases} \\ &3. \text{ prediction set: } \widehat{C}_{n}\left(X_{n+1}\right) = \Big\{ y \in \mathbb{R} : R_{n+1}^{y} \leq \mathcal{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_{i}^{y}}\right) \Big\}. \end{aligned}$ 

Drawback: a steep computational cost.

THEOREM:

 $\mathbb{P}\left\{ Y_{n+1} \in \widehat{C}_n\left(X_{n+1}\right) \right\} \geq 1 - \alpha \text{ holds true for both split conformal and full conformal.}$ 

## 1.3 Jackknife+

(close to cross-conformal prediction in Vovk (2013), offering a compromise between the computational and statistical costs)

- $1. \ \text{training data with $i$th point removed: } \\ \hat{\mu}_{-i} = \mathcal{A}\left(\left(X_1,Y_1\right),\ldots,\left(X_{i-1},Y_{i-1}\right),\left(X_{i+1},Y_{i+1}\right),\ldots,\left(X_n,Y_n\right)\right).$
- 2. residuals:  $R_{i}^{\mathrm{LOO}} = |Y_{i} \hat{\mu}_{-i}\left(X_{i}\right)|.$
- 3. prediction set:

$$\left[ \mathbf{Q}_{\alpha} \left( \sum_{i=1}^n \tfrac{1}{n+1} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) - R_i^{\mathsf{LOO}}} + \tfrac{1}{n+1} \cdot \delta_{-\infty} \right), \ \mathbf{Q}_{1-\alpha} \left( \sum_{i=1}^n \tfrac{1}{n+1} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) + R_i^{\mathsf{LOO}}} + \tfrac{1}{n+1} \cdot \delta_{+\infty} \right) \right]$$

Drawback: while in practice the it generally provides coverage close to the target level  $1-\alpha$ , its theoretical guarantee only ensures  $1-2\alpha$  probability of coverage in the worst case.

THEOREM:

 $\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n\left(X_{n+1}\right)\right\} \geq 1 - 2\alpha \text{ holds true for jackknife+}.$ 

# 2 Conformal time-series forecasting

Stankeviciute, M Alaa, and Schaar (2021): CF-RNNs

Multi-horizon time-series forecasting problem

#### **Notation:**

• the *i*th data point:  $Z_i = (y_{1:t}^{(i)}, y_{t+1:t+H}^{(i)})$ . Note that the label  $y_{t+1:t+H}^{(i)}$  is now an Hdimensional value, in contrast with the scalar y value from before.

### **Assumption:**

• exchangeable time-series observations

# 2.1 Methodology

(Split conformal prediction)

- 1. training set: train the underlying (auxiliary) model  $\hat{\mu}: \mathbb{R}^t \to \mathbb{R}^H$ , which produces multihorizon forecasts **directly** (conditionally independent predictions).
- 2. calibration set: obtain the H-dimensional nonconformity scores

$$R_i = \left[ \left| y_{t+1}^{(i)} - \hat{y}_{t+1}^{(i)} \right|, \dots, \left| y_{t+H}^{(i)} - \hat{y}_{t+H}^{(i)} \right| \right]^\top.$$

3. prediction set:  $\Gamma_1^{\alpha}\left(y_{(1:t)}^{(n+1)}\right), \dots, \Gamma_H^{\alpha}\left(y_{(1:t)}^{(n+1)}\right)$ , where  $\Gamma_h^{\alpha}\left(y_{(1:t)}^{(n+1)}\right) = \left[\hat{y}_{t+h}^{(n+1)} - \hat{\varepsilon}_h, \hat{y}_{t+h}^{(n+1)} + \hat{\varepsilon}_h\right]$ ,  $\forall h \in \{1, \dots, H\}$  with the critical nonconformity scores  $\hat{\varepsilon}_1, \dots, \hat{\varepsilon}_H$  become the  $\lceil (n+1)(1-\alpha/H) \rceil$ -th smallest residuals in the corresponding nonconformity score distributions. (Bonferroni correction)

#### THEOREM:

- $\mathcal{D} = \left\{ \left( y_{1:t}^{(i)}, y_{t+1:t+H}^{(i)} \right) \right\}_{i=1}^n$ : **exchangeable** time-series observations.  $\hat{\mu}$ : model predicting H-step forecasts using **the direct strategy**.

$$\mathbb{P}\left(\forall h \in \{1,\dots,H\} \cdot y_{t+h} \in [\hat{y}_{t+h} - \hat{\varepsilon}_h, \hat{y}_{t+h} + \hat{\varepsilon}_h]\right) \geq 1 - \alpha.$$

# 3 NexCP: Conformal prediction beyond exchangeability

Barber et al. (2023)

- 1. Nonexchangeable conformal with a **symmetric** algorithm (weights)
- 2. Nonexchangeable conformal with **nonsymmetric** algorithms (weights & swap)

#### 3.1 Notation

- the *i*th data point  $Z_i = (X_i, Y_i)$
- the full data sequence  $Z=(Z_1,\dots,Z_{n+1})$  the sequence after swap  $Z^i=(Z_1,\dots,Z_{i-1},Z_{n+1},Z_{i+1},Z_n,Z_i)$

# 3.2 Methodology

- 1. Choose fixed (non-data-dependent) weights  $w_1, \dots, w_n \in [0, 1]$  with the intuition that
- a higher weight should be assigned to a data point that is "trusted" more. 2. Normalize weights  $\tilde{w}_i = \frac{w_i}{w_1 + \dots + w_n + 1}, i = 1, \dots, n$  and  $\tilde{w}_{n+1} = \frac{1}{w_1 + \dots + w_n + 1}$ . 3. Generate "tagged" data points  $(X_i, Y_i, t_i) \in \mathcal{X} \times \mathbb{R} \times \mathcal{T}$ .
- 4. Swap data set, resulting in  $Z^K$  with  $K \sim \sum_{i=1}^{n+1} \tilde{w}_i \cdot \delta_i$ , i.e., two data points have swapped
- 5. Apply algorithm  $\mathcal{A}$  to  $Z^K$  in place of Z.

# 3.3 Split conformal prediction

• prediction set:  $\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm Q_{1-\alpha}\left(\sum_{i=1}^n \widetilde{w}_i \cdot \delta_{R_i} + \widetilde{w}_{n+1} \cdot \delta_{+\infty}\right)$ 

# 3.4 Full conformal prediction

- 1. training data & a hypothesized test point:  $\hat{\mu}^{y,k} = \mathcal{A}\left(\left(X_{\pi_k(i)}, Y_{\pi_k(i)}^y, t_i\right) : i \in [n+1]\right)$  for any  $y \in \mathbb{R}$  and  $k \in [n+1]$ , where  $\pi_k$  is the permutation on [n+1] swapping indices k
- and n+1, and  $Y_i^y = \begin{cases} Y_i, & i=1,\dots,n \\ y, & i=n+1 \end{cases}$ .

  2. residuals:  $R_i^{y,k} = \begin{cases} |Y_i \hat{\mu}^{y,k}(X_i)|, & i=1,\dots,n \\ |y \hat{\mu}^{y,k}(X_{n+1})|, & i=n+1 \end{cases}$ .
- 3. prediction set:  $\widehat{C}_n\left(X_{n+1}\right) = \left\{y: R_{n+1}^{y,K} \leq Q_{1-\alpha}\left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{R^{y,K}}\right)\right\}.$

#### THEOREM:

• Lower bounds on coverage.

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n\left(X_{n+1}\right)\right\} \geq 1 - \alpha - \sum_{i=1}^n \tilde{w}_i \cdot \mathrm{d_{TV}}\left(R(Z), R\left(Z^i\right)\right)$$

• Upper bounds on coverage.

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_{n}\left(X_{n+1}\right)\right\} < 1 - \alpha + \tilde{w}_{n+1} + \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathrm{d_{TV}}\left(R(Z), R\left(Z^{i}\right)\right),$$

if  $R_1^{Y_{n+1},K},\dots,R_n^{Y_{n+1},K},R_{n+1}^{Y_{n+1},K}$  are distinct with probability 1.

The results hold true for both nonexchangeable split conformal and full conformal.

So, if  $\tilde{w}_{n+1} = \frac{1}{w_1 + \dots + w_n + 1}$  is small (the effective sample size is large), then mild violations of exchangeability can only lead to mild undercoverage or to mild overcoverage.

# 3.5 Jackknife+

1. training data with ith point removed and data tag swapped:

$$\hat{\mu}_{-i}^k = \mathcal{A}\left(\left(X_{\pi_k(j)}, Y_{\pi_k(j)}, t_j\right) : j \in [n+1], \pi_k(j) \notin \{i, n+1\}\right).$$

- 2. residuals:  $R_i^{k,\text{LOO}} = |Y_i \hat{\mu}_{-i}^k(X_i)|$ .
- 3. prediction set:

$$\left[ \mathbf{Q}_{\alpha} \left( \sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}^{K}(X_{n+1}) - R_{i}^{K,\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{-\infty} \right), \ \mathbf{Q}_{1-\alpha} \left( \sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}^{K}(X_{n+1}) + R_{i}^{K,\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{+\infty} \right) \right]$$

THEOREM:

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n\left(X_{n+1}\right)\right\} \geq 1 - 2\alpha - \textstyle\sum_{i=1}^n \tilde{w}_i \cdot \mathrm{d_{TV}}\left(R_{\mathrm{jack}\;+}(Z), R_{\mathrm{jack}\;+}\left(Z^i\right)\right)$$

# 4 WCP: Conformal prediction under covariate shift

Tibshirani et al. (2019)

A weighted version of conformal prediction, using a quantile of a suitably weighted empirical distribution of nonconformity scores.

# 4.1 Setup/assumption - Covariate shift

Focus on settings in which the data  $(X_i, Y_i)$ , i = 1, ..., n + 1 are no longer exchangeable. Specifically,

$$\begin{split} &(X_i,Y_i) \overset{\text{i.i.d.}}{\sim} \ P = P_X \times P_{Y|X}, \quad i = 1,\dots,n, \\ &(X_{n+1},Y_{n+1}) \sim \widetilde{P} = \widetilde{P}_X \times P_{Y|X}, \text{ independently.} \end{split}$$

the test and training covariate distributions differ, but the likelihood ratio between the two distributions,  $d\widetilde{P}_X/dP_X$ , must be known exactly or well approximated for correct coverage.

# 4.2 Methodology

#### **Prediction set:**

$$\bullet \ \text{CP: } \widehat{C}_{n}\left(X_{n+1}\right) = \widehat{\mu}\left(X_{n+1}\right) \pm \mathbf{Q}_{1-\alpha}\left(\textstyle\sum_{i=1}^{n}\frac{1}{n+1}\cdot\delta_{R_{i}} + \frac{1}{n+1}\cdot\delta_{+\infty}\right).$$

• NexCP: 
$$\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm Q_{1-\alpha}\left(\sum_{i=1}^n \widetilde{w}_i \cdot \delta_{R_i} + \widetilde{w}_{n+1} \cdot \delta_{+\infty}\right).$$

$$-$$
 weights  $w$  are fixed

– 
$$\tilde{w}_i = \frac{w_i}{w_1+\cdots+w_n+1}, i=1,\ldots,n$$
 and  $\tilde{w}_{n+1} = \frac{1}{w_1+\cdots+w_n+1}$ 

• WCP: 
$$\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm Q_{1-\alpha}(\sum_{i=1}^n p_i^w(x)\delta_{R_i} + p_{n+1}^w(x)\delta_{\infty}).$$

$$\begin{array}{l} -\ w = \mathrm{d}\widetilde{P}_X/\mathrm{d}P_X \text{ or } w \propto \mathrm{d}\widetilde{P}_X/\mathrm{d}P_X \\ -\ p_i^w(x) = \frac{w(X_i)}{\sum_{j=1}^n w(X_j) + w(x)}, i = 1, \dots, n, \text{ and } p_{n+1}^w(x) = \frac{w(x)}{\sum_{j=1}^n w(X_j) + w(x)} \end{array}$$

The weight function  $\hat{w}$  can be estimated using logistic regression, random forests, etc.

#### THEOREM:

Assume data from the model Equation 1. Assume  $\widetilde{P}_X$  is absolutely continuous with respect to  $P_X$ , and denote  $w=\mathrm{d}\widetilde{P}_X/\mathrm{d}P_X$ . For any score function S, and any  $\alpha\in(0,1)$ , define for  $x\in\mathbb{R}^d$ . Then

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

# 4.3 Comparison to NexCP

- 1. Assumption
  - WCP: covariate shift
  - NexCP: do not make any assumption on the joint distribution of the n+1 points
- 2. Weights
  - WCP: a function of the data point  $(X_i,Y_i)$  to compensate for the **known** distribution shift.
  - NexCP: required to be fixed, can compensate for **unknown** violations of the exchangeability assumption, as long as the violations are **small** (to ensure a low coverage gap).
- 3. Nonsymmetric algorithm
  - WCP: No.
  - NexCP: Yes.
- 4. For exchangeable data

- WCP: does not have any coverage guarantee.
- NexCP: retains exact coverage.

# 5 ACP: Adaptive conformal inference under distribution shift

Gibbs and Candes (2021)

- No assumptions on the data-generating distribution.
- Modelling the distribution shift as a learning problem in a single parameter whose optimal value is varying over time and must be continuously re-estimated.
- Adjust significance level  $\alpha$  based on rolling coverage of  $Y_t$  .

## 5.1 Methodology

Work with score function  $S(\cdot)$  and quantile function  $\hat{Q}(\cdot)$ .

#### Some facts:

- If the distribution of the data is shifting over time, both functions should be regularly re-estimated to align with the most recent observations.
- The realized miscoverage rate  $M_t(\alpha)$  also varies over time and may not be equal or close to  $\alpha$ .

#### **Assumptions:**

Assume that there may be an alternative value  $\alpha^* \in [0,1]$  such that  $M_t(\alpha^*) \cong \alpha$ .

Assume that with probability one,  $\hat{Q}_t(\cdot)$  is continuous, non-decreasing and such that  $\hat{Q}_t(0) = -\infty$  and  $\hat{Q}_t(1) = \infty$ .

### Adaptive conformal inference:

- Under assumptions,  $M_t(\cdot)$  will be non-decreasing on [0,1] with  $M_t(0)=0$  and  $M_t(1)=1$ .
- Define  $\alpha_t^* := \sup \{ \beta \in [0,1] : M_t(\beta) \le \alpha \}$ , then  $M_t(\alpha_t^*) = \alpha$ .
- Use a simple **update process** to perform the calibration.
  - Intuition: after examining the empirical miscoverage frequency of the previous prediction sets, decreasing (increasing) estimate of  $\alpha_t^*$  if the prediction sets were historically under-covering (over-covering)  $Y_t$ .

– Let  $\alpha_1 = \alpha$ , consider the **update** 

$$\alpha_{t+1} := \alpha_t + \gamma \left(\alpha - \operatorname{err}_t\right)$$

OR

$$\alpha_{t+1} = \alpha_t + \gamma \left( \alpha - \sum_{s=1}^t w_s \operatorname{err}_s \right),$$

where  $\gamma > 0$  is a fixed step size parameter whose choice gives a tradeoff between adaptability and stability.

So the distribution is allowed to shift continuously over time.

#### THEOREM:

With probability one we have that for all  $T \in \mathbb{N}$ ,

$$\left|\frac{1}{T}\sum_{t=1}^{T}err_{t}-\alpha\right|\leq\frac{\max\left\{\alpha_{1},1-\alpha_{1}\right\}+\gamma}{T\gamma}.$$

In particular,  $\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^T err_t \overset{\text{a.s.}}{=} \ \alpha.$ 

# 6 PID: Conformal PID control for time series prediction

Angelopoulos, Candes, and Tibshirani (2023)

- PID: proportional-integral-derivative (control theory).
- reactive + forward-looking.

## 6.1 Methodology

The proposed conformal PID controller is given by

$$q_{t+1} = \underbrace{\eta(\operatorname{err}_t - \alpha)}_{\mathbf{P}} + \underbrace{r_t\left(\sum_{i=1}^t (\operatorname{err}_i - \alpha)\right)}_{\mathbf{I}} + \underbrace{g_t'}_{\mathbf{D}}.$$

The goal is to achieve **long-run coverage** in time, i.e.,  $\frac{1}{T} \sum_{t=1}^{T} \operatorname{err}_{t} = \alpha + o(1)$ , where o(1) denotes a quantity that tends to zero as  $T \to \infty$ .

- P: Quantile tracking. ACI can be regarded as a special case but it can sometimes output infinite or null prediction sets, while quantile tracking on the scale of the original score sequence does not have this behavior.
- I: Error integration.  $r_t$  should be a saturation function to achieve long-run coverage.
- D: Scorecasting (forward-looking). It trains a second model to predict the quantile of the next score.

Reparametrize the PID formula to produce a sequence of quantile estimates  $q_t, t \in N$  used in the prediction sets:

let  $\hat{q}_{t+1}$  be any function of the past:  $x_i, y_i, q_i$ , for  $i \leq t$ , then update

$$q_{t+1} = \underbrace{\hat{q}_{t+1}}_{\text{scorecaster}} + \underbrace{r_t \left( \sum_{i=1}^t (\text{err}_i - \alpha) \right)}_{\text{integrator}},$$

which is generally useful and is the main focus of the paper.

The applications only consider one-step-ahead forecast.

# 7 Others

#### 7.1 EnbPI: predictive inference method around ensemble estimators

Xu and Xie (2021)

- For Dynamic time series
- Ensemble point forecasts + update residuals

## 7.2 SPCI: Sequential Predictive Conformal Inference

Xu and Xie (2023)

• Adaptively re-estimate the conditional quantile of non-conformity scores, upon leveraging the temporal dependency among residuals. Random Forest for quantile regression is used.

# 7.3 Kath & Ziel (2021, IJF)

Kath and Ziel (2021)

#### Method 1.

The steps are:

- 1. Re-arrange time series data as form  $Z = \{(x_1, y_1), \dots, (x_L, y_L)\}.$
- 2. Randomly split observations into subsets  $\pi$  (training set) and  $1-\pi$  (calibration set).
- 3. Train a random forecast model using the training set and generate out-of-sample forecasts.
- 4. Calculate non-conformity score.
- 5. Obtain final prediction interval estimation.

#### Method 2.

The differences compared to Method 1 are:

- 1. Here an adjusted normalized non-conformity score  $\lambda_{i,h}=\frac{|y_{i,h}-\hat{y}_{i,h}|}{|\hat{\varepsilon}_{i,h}|}$  is used.
- 2. A second explicit error estimation model is trained to estimate the error associated with the prediction  $\hat{y}_{t,h}$ , i.e.,  $\varepsilon_{t,h}$ .
- 3. The new interval forecast is now given by  $y_{\alpha,T+1,h} = \hat{y}_{T+1,h} \pm \lambda_{L+1,h}^{\alpha} |\hat{\varepsilon}_{L+1,h}|$ .

The applications only consider one-step-ahead forecast.

## 7.4 TimeGPT

Garza and Mergenthaler-Canseco (2023)

For uncertainty quantification, they perform rolling forecasts on the latest available data to estimate the model's errors in forecasting the particular target time series.

The h-step-ahead forecast is generated based on h-step-ahead non-conformity errors on the calibration set separately.

# 7.5 LCP: Localized conformal prediction

### Guan (2022)

The **weight** on data point i is determined as a function of the distance  $||X_i - X_{n+1}||_2$ , to enable predictive coverage that holds **locally** (in neighborhoods of X space, that is, an approximation of prediction that holds conditional on the value of  $X_{n+1}$ ).

# 8 Simulation

## 8.1 Setup

Simulate a time series y with length T=5000 from an AR(2) model with  $\phi_1=0.8,\,\phi_2=-0.5,$  and  $\sigma^2=1.$ 

Only consider one-step-ahead forecasting, i.e., h = 1.

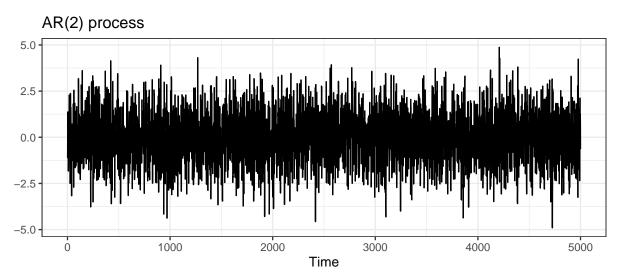


Figure 1: Simulated time series from an AR(2) model.

## 8.2 Split conformal prediction with fixed training set

#### 8.2.1 Details

Let n be the number of data used to fit an AR(2) model, and m be the number of data in the calibration set.

- Step 1. Rearrange the time series as  $Z_i=(X_i,Y_i)$ , where  $X_i=y_{i:(i+1)}$  and  $Y_i=y_{i+2}$ ,  $i=1,2,\ldots,T-2$ .
- Step 2. Train an AR(2) model  $\hat{\mu}$  based on training set with length  $n, Z_{tr} = (Z_1, Z_2, \dots, Z_n)$ .
- Step 3. Calculate nonconformity scores (absolute residuals) based on calibration set with length m, i.e.,  $R_i = |Y_i \hat{\mu}(X_i)|$ ,  $i = n + 1, n + 2, \dots, n + m$ .
- Step 4. Generate PI on test set.  $\hat{C}_m(X_i) = \hat{\mu}(X_i) \pm \mathbf{Q}_{1-\alpha} \left(\sum_{j=n+1}^{n+m} w_j \cdot \delta_{R_j} + w_i \cdot \delta_{+\infty}\right)$  for  $i=n+m+i,\ldots,T-2$ .

## 8.2.2 Results

Let n = m = 500 and fit the AR(2) model using the 1m function.

Consider methods: CP, WCP.LR, WCP.RF, NexCP with  $\alpha = 0.1$ .

Issues:

- PIs have constant width over the test set. We can generate PIs with varying local width by using a function to perform training on the absolute residuals i.e., to produce an estimator of E(R|X).
- When generating weights via GLM or RF in WCP method, we need to use all data from the test set, which is not reasonable.
- Regression-based model.

## 8.3 Split conformal prediction with rolling training set

#### 8.3.1 Details

Let n be the number of observations used to fit an AR(2) model, and m be the number of observations in the calibration set.

For i = n + 1, n + 2, ..., T:

- Step 1. Fit an AR(2) model  $\hat{\mu}_{i-1}$  based on observations  $y_{(i-n):(i-1)}$ , generate one-step-ahead forecast  $\hat{y}_i$ .
- When i > n + m:
  - Step 2. Calculate weights for the updated calibration set with length m and the updated test set with length 1 using different methods. Here WCP can not be applied because we only have a test set with length equal to one.

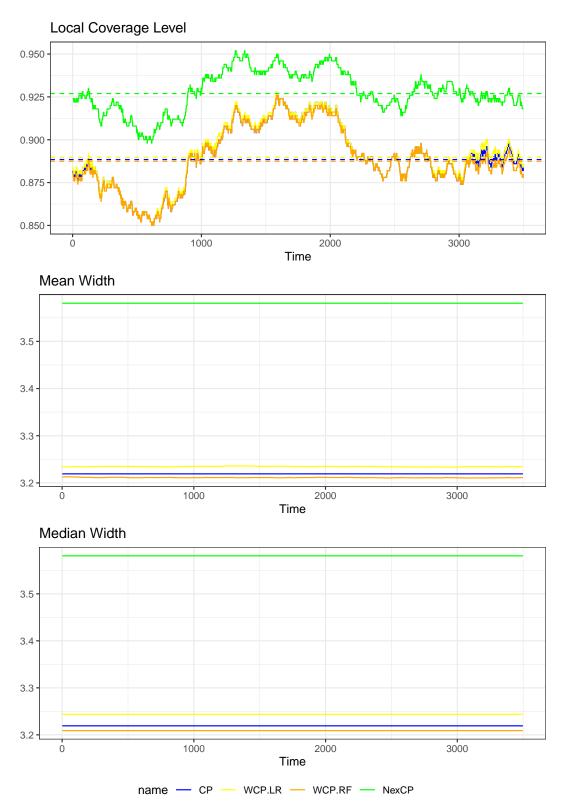


Figure 2: Local coverage frequencies and width for split conformal prediction methods with fixed training set (k=500).

- Step 3. Generate PI on test set.  $\hat{y}_i \pm \mathbf{Q}_{1-\alpha} \left( \sum_{j=i-m}^{i-1} w_i \cdot \delta_{R_j} + w_i \cdot \delta_{+\infty} \right)$ .
- Setp 4 for ACP. Update  $\alpha$  based on the recent empirical miscoverage frequency.
- Step 5. Calculate nonconformity scores (absolute residuals)  $R_i = |y_i \hat{y}_i|$ .

#### 8.3.2 Results

Let n=m=500 and fit AR(2) models using the Arima function with setting order = c(2,0,0), include.mean = TRUE, method = "CSS" to make it comparable with the previous result.

Consider methods: AR, CP, NexCP, ACP, PID with  $\alpha = 0.1$ .

For the PID method:

- The AR(2) models are trained using nfit observations through a rolling window strategy, as with the other methods.
- Theta method is used as the scorecaster to forecast the conformity scores. An expanding window strategy is used if ncast = NULL; a rolling window strategy is used if ncast != NULL (here we use rolling windows with ncast = ncal for comparison with other methods).
- The first nburnin outputs are removed to have output of equal length. (nburnin is equal to ncal in other methods.)

#### Features:

- The fitted model is updating over time.
- PIs have changing width over the test set.
- Other non-regression-based models can be considered.
- Time-consuming because of the rolling window approach (but is still very quick for this simulation).

# 9 To do list

| ☐ Generalize the existing methods and get a general function for implementation.             |
|--|
| ☐ Symmetric/asymmetric scores.   |
| ☐ Expanding/rolling window strategy.   |
| $\square$ Include weights in PID.  |
| $\square$ Handle seasonal time series and specify methods used for forecasting and scorecast |
| ing.   |
| ☐ Multi-step ahead forecasting.  |

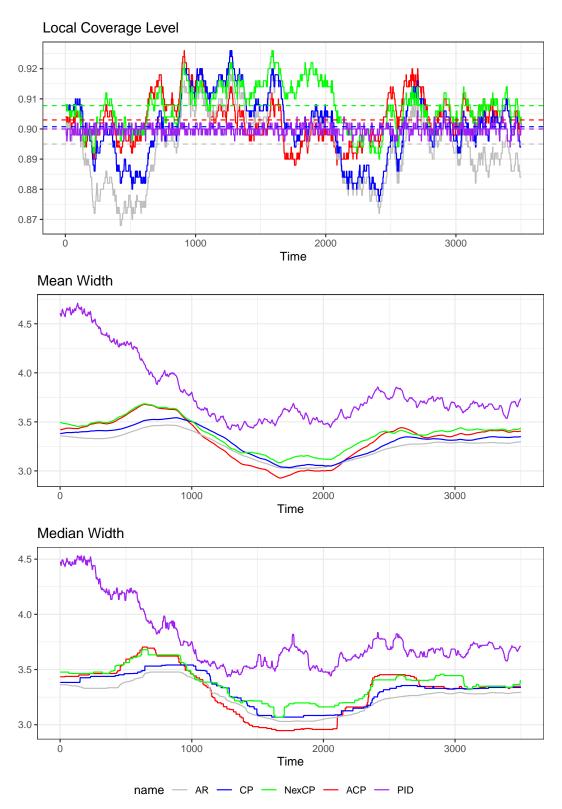


Figure 3: Local coverage frequencies and width for split conformal prediction methods with rolling training set and calibration set (k=500).

| ☐ Correlation between multi step ahead residuals. |
|---|
| $\square$ Similar strategy as PID.                |
| More simulations and real-world data.             |
| Theoretical proof.                                |
| Other data-dependent weight.                      |
| Hierarchical time series?                         |

# 10 References

- Angelopoulos, Anastasios N, Emmanuel J Candes, and Ryan J Tibshirani. 2023. "Conformal PID Control for Time Series Prediction." arXiv Preprint arXiv:2307.16895.
- Barber, Rina Foygel, Emmanuel J. Candès, Aaditya Ramdas, and Ryan J. Tibshirani. 2023. "Conformal Prediction Beyond Exchangeability." *The Annals of Statistics* 51 (2). https://doi.org/10.1214/23-aos2276.
- Garza, Azul, and Max Mergenthaler-Canseco. 2023. "TimeGPT-1." arXiv Preprint arXiv:2310.03589.
- Gibbs, Isaac, and Emmanuel Candes. 2021. "Adaptive Conformal Inference Under Distribution Shift." Advances in Neural Information Processing Systems 34: 1660–72.
- Guan, Leying. 2022. "Localized Conformal Prediction: A Generalized Inference Framework for Conformal Prediction." *Biometrika* 110 (1): 33–50. https://doi.org/10.1093/biomet/asac040.
- Kath, Christopher, and Florian Ziel. 2021. "Conformal Prediction Interval Estimation and Applications to Day-Ahead and Intraday Power Markets." *International Journal of Forecasting* 37 (2): 777–99.
- Shafer, Glenn, and Vladimir Vovk. 2008. "A Tutorial on Conformal Prediction." *Journal of Machine Learning Research* 9 (3).
- Stankeviciute, Kamile, Ahmed M Alaa, and Mihaela van der Schaar. 2021. "Conformal Time-Series Forecasting." Advances in Neural Information Processing Systems 34: 6216–28.
- Tibshirani, Ryan J, Rina Foygel Barber, Emmanuel Candes, and Aaditya Ramdas. 2019. "Conformal Prediction Under Covariate Shift." Advances in Neural Information Processing Systems 32.
- Vovk, Vladimir. 2013. "Cross-Conformal Predictors." Annals of Mathematics and Artificial Intelligence 74 (1-2): 9–28. https://doi.org/10.1007/s10472-013-9368-4.
- Vovk, Vladimir, Alexander Gammerman, and Glenn Shafer. 2005. Algorithmic Learning in a Random World. Springer-Verlag. https://doi.org/10.1007/b106715.
- Xu, Chen, and Yao Xie. 2021. "Conformal Prediction Interval for Dynamic Time-Series." In *International Conference on Machine Learning*, 11559–69. PMLR.
- ——. 2023. "Sequential Predictive Conformal Inference for Time Series." In *International Conference on Machine Learning*, 38707–27. PMLR.