FACULTY OF ENGINEERING AND ARCHITECTURE

13th Symposium on Conformal and Probabilistic Prediction with Applications

Conformal Predictive Systems under Covariate Shift

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Overview

Introduction

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Conformal predictive systems

What?

- Conformal predictive systems (CPSs) output conformal predictive distributions
  - p-values arranged into a non-parametric distribution
- CPS = smooth conformal transducer $\cap$ randomized predictive system (RPS)
- Can be used to calibrate a probabilistic regression model (deterministic prediction system)
- Probabilistically calibrated

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- Probabilistically calibrated

Assumptions

- General IID model

Conformal predictive systems

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  - p-values arranged into a non-parametric distribution
- CPS = smooth conformal transducer $\cap$ randomized predictive system (RPS)
- Can be used to calibrate a probabilistic regression model (deterministic prediction system)
- Probabilistically calibrated

Assumptions

- General IID model

Why?

- Decision-making
- Results into a central conformal predictor
- ...

IID assumption violated?

Consequences

- Losing validity guarantees

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When?

- Covariate shift
  - causal inference
  - time series
  - scientific discovery
  - transfer learning
- Label shift
  - time series
  - ...

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Remdy

- Conformal prediction (CP)
  - weighted CP (Tibshirani et al., 2019)
  - (Dt) Adaptive conformal inference (Gibbs and Candes, 2021; Gibbs and Candès, 2024)
  - ...
- CPS?

IID assumption violated?

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When?

- Covariate shift
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- Conformal prediction (CP)
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  - (Dt) Adaptive conformal inference (Gibbs and Candes, 2021; Gibbs and Candès, 2024)
  - ...
- CPS?
  - **weighted CPS** (this work)
    - validity under covariate shift

Conformal Predictive System

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Randomized predictive system

Definition (Randomized predictive system (RPS), Vovk et al., 2019)

A function $Q : \mathbf{Z}^{n+1} \times [0,1] \to [0,1]$ is an RPS:

R1.1 The function $Q(z_1, ..., z_n, (x_{n+1}, y), \tau)$ is monotonically increasing both in y and τ.

R1.2 For each $\tau, \tau' \in [0,1]$, $Q(z_1, ..., z_n, (x_{n+1}, y), \tau) \geq Q(z_1, ..., z_n, (x_{n+1}, y'), \tau')$ if $y > y'$,

R1.3 $\lim_{y \to -\infty} Q(z_1, ..., z_n, (x_{n+1}, y), 0) = 0, \qquad \lim_{y \to \infty} Q(z_1, ..., z_n, (x_{n+1}, y), 1) = 1$

R2 When $z_1 \sim P, ..., z_n \sim P, z_{n+1} \sim P$, and $\tau \sim \mathit{Uniform}(0,1)$, all assumed to be independent, the distribution of Q is uniform:

$$\forall \alpha \in [0,1] : \mathbb{P}\{Q(z_1, ..., z_n, z_{n+1}, \tau) \leq \alpha\} = \alpha$$

Smooth conformal transducer

Definition (Smooth conformal transducer, Vovk et al., 2022)

The conformal transducer determined by a conformity measure A is defined as,

$$Q(z_1, ..., z_n, (x_{n+1}, y), \tau) := \sum_{i=1}^{n+1} [R_i^y < R_{n+1}^y] \frac{1}{n+1} + \sum_{i=1}^{n+1} [R_i^y = R_{n+1}^y] \frac{\tau}{n+1}$$

where $(z_1, ..., z_n)$ is the training sequence, $\tau \in [0, 1]$, x_{n+1} is a test object, and for each label y the corresponding conformity score R_i^y is defined as

$$\begin{aligned} R_i^y &:= A(z_1, ..., z_{i-1}, z_{i+1}, ..., z_n, (x_{n+1}, y), z_i), \qquad i = 1, ..., n \\ R_{n+1}^y &:= A(z_1, ..., z_n, (x_{n+1}, y)). \end{aligned}$$

CPS = conformal transducer $\cap$ RPS

- For smooth conformal transducers: $Q(z_1, ..., z_n, z_{n+1}, \tau) \sim Uniform(0, 1)$
  - coincides with R2 of RPS
  - under IID assumption
- To satisfies R1.1 and R1.3, the conformal transducer can only be defined by certain conformity measures A
  - monotonic conformity measures (e.g., $\alpha_i := y_i - \hat{y}_i$)

Weighted Conformal Predictive System

Problem setting: covariate shift

A covariate shift is a distributional shift where the test object (x_{n+1}, y_{n+1}) is differently distributed, i.e. $x_{n+1} \sim \tilde{P}_X$, than the training data $z_i = (x_i, y_i), i = 1, ..., n$ where $x_i \sim P_X$, thus $\tilde{P}_X \neq P_X$. However, the relationship between inputs and labels remains fixed.

$$
\begin{aligned}
(x_i, y_i) &\overset{\text{iid}}{\sim} P = P_X \times P_{Y|X}, \quad i = 1, ..., n \\
(x_{n+1}, y_{n+1}) &\sim \tilde{P} = \tilde{P}_X \times P_{Y|X}
\end{aligned}
$$

Weighted conformal predictive system

- Provides probabilistic calibrated predictive distributions under covariate shift
- Builds on the same idea as weighted CP Tibshirani et al., 2019.
  - Weight each conformity score by a probability proportionally to the likelihood ratio $w(x_i) = \frac{d\tilde{P}_X(x_i)}{dP_X(x_i)}$
- Weighted CPS = Smooth weighted conformal transducer $\cap$ Weighted RPS

Smooth weighted conformal transducer

Definition (Smooth weighted conformal transducer)

The weighted conformal transducer determined by conformity measure A and likelihood ratio $w(x_i) = \frac{d\tilde{P}_X(x_i)}{dP_X(x_i)}$ is defined as,

$$Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau) := \sum_{i=1}^{n+1} [R_i^y < R_{n+1}^y] p_i^w(x) + \sum_{i=1}^{n+1} [R_i^y = R_{n+1}^y] p_i^w(x) \tau$$

where

$$p_i^w(x) = \frac{w(x_i)}{\sum_{j=1}^n w(x_j) + w(x)}, \qquad p_{n+1}^w(x) = \frac{w(x)}{\sum_{j=1}^n w(x_j) + w(x)}.$$

Weighted randomized predictive system

Definition (Weighted randomized predictive system (WRPS))

A function $Q : \mathbf{Z}^{n+1} \times [0,1] \to [0,1]$ is an WRPS:

R1.1 The function $Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau)$ is monotonically increasing both in y and τ.

R1.2 For each $\tau, \tau' \in [0,1]$, $Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau) \geq Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y'), \tau')$ if $y > y'$,

R1.3 $\lim_{y \to -\infty} Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), 0) = 0$,
$\lim_{y \to \infty} Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), 1) = 1$,

R2 When $z_1 \sim P, ..., z_n \sim P$, $z_{n+1} \sim \tilde{P}$, and $\tau \sim Uniform(0,1)$, all assumed to be independent, the distribution of Q is uniform:

$$\forall \alpha \in [0,1] : \mathbb{P}\{Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, z_{n+1}, \tau) \leq \alpha\} = \alpha$$

WCPS = weighted conformal transducer ∩ WRPS

- To satisfies R1.1 and R1.3, the weighted conformal transducer can only be defined by certain conformity measures A.
  - monotonic conformity measures (e.g., $\alpha_i := y_i - \hat{y}_i$)
  - proof similar to CPS
- For smooth weighted conformal transducers: $Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, z_{n+1}, \tau) \sim Uniform(0, 1)$
  - coincides with R2 of WRPS
  - under covariate shift assumption and knowing $w(x_i) = \frac{d\tilde{P}_X(x_i)}{dP_X(x_i)}$
  - proof not provided yet

Weighted split conformal predictive system

We can also extend the computationally efficient split conformal predictive system by introducing a smooth weighted split conformal transducer.

Definition (Smooth weighted split conformal transducer)

The weighted split conformal transducer determined by conformity measure A and likelihood ratio $w(x_i) = \frac{d\tilde{P}_X(x_i)}{dP_X(x_i)}$ is defined as,

$$Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau) := \sum_{i=m+1}^{n} [R_i < R^y] p_i^w(x) + \sum_{i=m+1}^{n} [R_i = R^y] p_i^w(x)\tau + p_{n+1}^w(x)\tau$$

where

$$p_i^w(x) = \frac{w(x_i)}{\sum_{j=1}^{n} w(x_j) + w(x)}, \qquad p_{n+1}^w(x) = \frac{w(x)}{\sum_{j=1}^{n} w(x_j) + w(x)}.$$

Experiments

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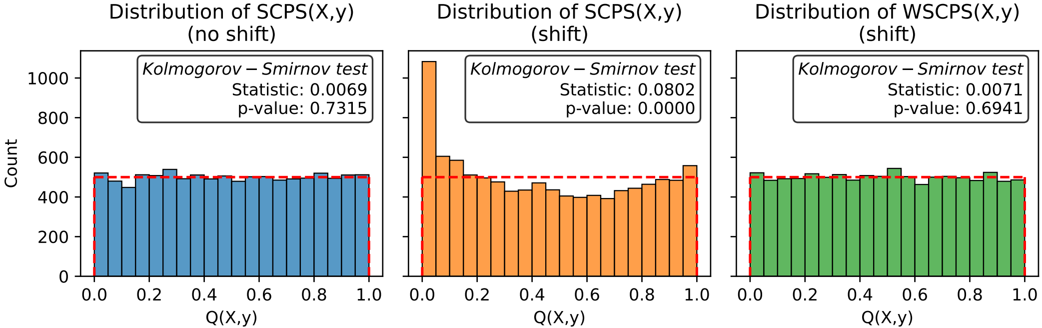
Setup

From Kang and Schafer, 2007, also used in Yang et al. (2022), where each observation i is generated in the following way:

- $(x_{i1}, x_{i2}, x_{i3}, x_{i4})^T$ is independently distributed as $N(0, I_4)$ where I_4 represents the 4×4 identity matrix.
- $y_i = 210 + 27.4x_{i1} + 13.7x_{i2} + 13.7x_{i3} + 13.7x_{i4} + \varepsilon_i, \quad \text{where} \quad \varepsilon_i \sim N(0, 1)$
- $w(x) = \exp(-x_{i1} + 0.5x_{i2} - 0.25x_{i3} - 0.1x_{i4})$, which represents the likelihood ratio of the covariate distributions of the shifted test set D_{test} and training set D_{train}.

Probabilistic calibration under covariate shift

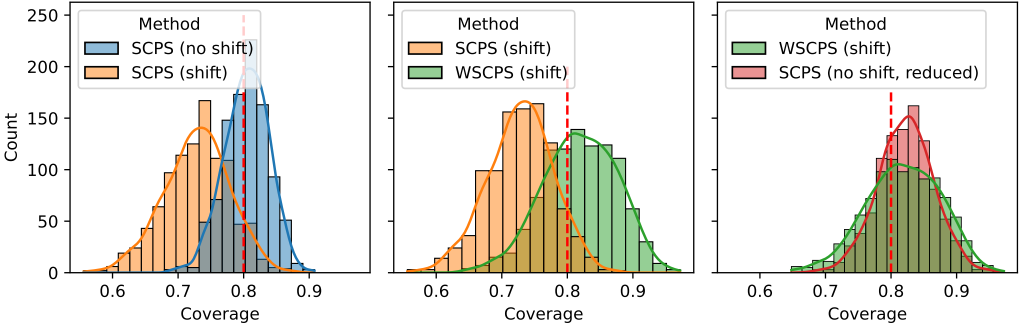


Intervals are still possible ...

$$C_{n+1}(x_{n+1}) := \left\{ y \in \mathbb{R} | \quad Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau) \in [\alpha, 1 - \alpha] \right\}$$

Intervals are still possible ...

$$C_{n+1}(x_{n+1}) := \left\{ y \in \mathbb{R} \middle| \quad Q(z_1, ..., z_n, \frac{d\tilde{P}}{dP}, (x_{n+1}, y), \tau) \in [\alpha, 1-\alpha] \right\}$$



crepes-weighted

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crepes-weighted: crepes made weighted

- Conformal prediction (regression, Tibshirani et al., 2019)
- Conformal prediction (classification)
- Conformal predictive systems (this work)
- See: https://github.com/predict-idlab/crepes-weighted

SCAN ME

crepes-weighted: crepes made weighted

```python
from sklearn.ensemble import RandomForestRegressor
from crepes_weighted import WrapRegressor

rf_wcps = WrapRegressor(RandomForestRegressor(n_estimators=100,
    random_state=17))
rf_wcps.fit(X_train_prop, y_train_prop)

```

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from sklearn.ensemble import RandomForestRegressor
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rf_wcps = WrapRegressor(RandomForestRegressor(n_estimators=100,
    random_state=17))
rf_wcps.fit(X_train_prop, y_train_prop)

rf_wcps.calibrate(X_cal, y_cal, likelihood_ratios=
    shifted_likelihood_cal, cps=True)

```

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from sklearn.ensemble import RandomForestRegressor
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rf_wcps.calibrate(X_cal, y_cal, likelihood_ratios=
    shifted_likelihood_cal, cps=True)

int_wcps = rf_wcps.predict_int(X_test[idx_shift], y=y_test[idx_shift],
    likelihood_ratios=shifted_likelihood_test[idx_shift])
```

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int_wcps = rf_wcps.predict_int(X_test[idx_shift], y=y_test[idx_shift], likelihood_ratios=shifted_likelihood_test[idx_shift])
dist_wcps = rf_wcps.predict_cps(X_test, y=y_test, likelihood_ratios=shifted_likelihood_test, return_cpds=True)
```

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    likelihood_ratios=shifted_likelihood_test[idx_shift])
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    shifted_likelihood_test, return_cpds=True)
p_values_wcps = rf_wcps.predict_cps(X_test, y=y_test, likelihood_ratios
    =shifted_likelihood_test)
```

crepes-weighted: crepes made weighted

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from sklearn.ensemble import RandomForestRegressor
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rf_wcps.fit(X_train_prop, y_train_prop)

rf_wcps.calibrate(X_cal, y_cal, likelihood_ratios=shifted_likelihood_cal, cps=True)

int_wcps = rf_wcps.predict_int(X_test[idx_shift], y=y_test[idx_shift], likelihood_ratios=shifted_likelihood_test[idx_shift])
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p_values_wcps = rf_wcps.predict_cps(X_test, y=y_test, likelihood_ratios=shifted_likelihood_test)
```

Conclusion

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- Successfully extended CPS to handle covariate shift
  - by introducing WCPS/WSCPS
- Practical implementation available via open-source Python package

Future work

- Formal proofs of theoretical conjectures
- Application to counterfactual inference
- Making CPS more conditionally probabilistically calibrated
- Weighted full CPS to `crepes-weighted`
- Dealing with prior (likelihood ratio)
  - imprecise probabilities, ...

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