Learning calibrated belief functions from conformal predictions Vitor Martin Bordini, Sebastien Destercke and Benjamin Quost CNRS, UMR 7253 Heudiasyc, UTC







Problem

- Common problem on machine learning predictions: poor calibration.
- Calibration definition: The level of confidence actually reflects the chance that the associated output turns out to be true.

 $\hat{P}(Y|X) \neq P(Y|X)$

- Inductive Conformal Prediction (ICP) [1] is a possible solution to this problem.
- What is the relation (if any) between ICPs and Belief Functions?

 H_1

 H_2

Possibility theory

• Possibility distribution: $\pi : \Omega \mapsto [0, 1]$

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- Necessity Measure *N* and Possibility Measure Π (equivalent to Belief and Plausibility Functions, respectively): $\Pi(B) = 1 - N(B^C) = \max_{x \in B} \pi(x), B \subseteq \Omega$.
- Limitation: we can only extract imprecise probabilities from a possibility distribution.

• α -cut: $\pi_{\alpha} = \{x \in \mathbb{R} | \pi(x) > \alpha\}[2].$

Inductive Conformal Prediction

- Dataset $Z = \{(x_i, w_i), w_i \in \Omega | i = 1, ..., n\}$ is exchangeable.
- Compute non-conformity scores α_i .
- Computes p-values, ICP output, by comparing the non-conformity scores of a single exemple and the ones of the calibration set.
- P-values property: $P(\{p(w_i) \le \delta\}) \le \delta, w_i \in \Omega$.
- In the exemple below, y_1 is a better prediction than y_2 because $p_{y_1} > p_{y_2}$.
- Advantages: Simple to implement/understand and with a rigorous theory behind it.
- Drawbacks: Calibration set (needs more data) and significantly slower.

$lpha_1$	α_{y_1}	$lpha_2$	$lpha_3$	α_{y_2}	$lpha_4$	
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Our solution

- Our hypothesis: ICP outputs can be learned directly from a machine learning model.
- We need p-values as labels, which doesn't exist in any public datasets.
- We train a model that estimates probability distributions and then we apply the ICP on this model output to compute p-values.
- This p-values are the labels to train a regressor.
- P-value vector p can be interpreted as a possibility distribution π .
- Estimation of calibrated belief functions via possibility distribution.

- Property: $P(\pi_{\alpha}) \ge 1 \alpha$.
- In the example below, we can compute the mass functions as $m(\{y_1\}) = p_{y_1} p_{y_2}$ and $m(\{y_1, y_2\}) = p_{y_2}.$

 p_{y_2} y_2 label y_1

Experiments

- CIFAR-10 dataset.
- Classifier: Fitnet backbone [3] + softmax layer.
- Regressor: Fitnet backbone + linear layer with activation function $\phi(x) = \frac{e^{x_i}}{\max_{x_i \in x} e^{x_i}}$.
- $\pi(\emptyset) = 0.$
- Training parameters: batch size 25, learning rate 0.001, momentum 0.9 and an Adam optimizer.

P-values comparison

- Comparison between ICP and the regressor outputs.
- Calibration dataset = 10% of the test dataset.
- The Mean Square Root(MSR) and the R2 coefficient are 0.02 and 0.8, respectively.
- Output averaged by the number of classes.
- Results for 200 outputs. Ideal result = Blue line.





Calibration size influence

- Goal = Change the calibration set size from 10 to 1000 instances and check how the accuracy of ICP and our algorithm grows.
- Regressor performs slightly worse after 100 instances, at most 2.5% below than the ICP, but has a better performance with less data.





Conclusion

- Calibration techniques make model predictions statistically valid.
- The ICP is a popular calibration technique but it is slower and requires more data.
- Our algorithm decrease the dependence of ICP on the calibration dataset while also being less computationally expensive and having similar performance.
- However, it still requires a minimum amount of data and takes more time to learn.
- Future works may solve this problem using co-learning techniques[4][5].

References

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