A Short Introduction to Conformal Prediction

Adrian Galdran, MSC Research Fellow
CVC Barcelona, Spain | Universitat Pompeu Fabra, Barcelona, Spain

Contents

1. Introduction: Uncertainty Formats

Note: Let us think of classification for simplicity today

Up to now, we have seen lots of alternatives to model uncertainty:

- **Leave Dropout turned on in test time.**
- **Multiple forward passes with $\neq$ data augmentations.**
- **Train several independent models, or using data subsets.**
- **Collect model snapshots during training.**
- **...**

But, after choosing one, how do we convey uncertainty info to a user?

1. Introduction: Uncertainty Formats

We could have:

- **A stochastic mechanism that, when sampled, returns different solutions, matching reality (a.k.a. Posterior Distribution)**

  Let the user sample the mechanism, or return mean +/ variance

- **A well-calibrated model**

  Just return its output = "confidence"

- **What about returning a subset of likely correct categories?**

2. Conformal Prediction: Vocabulary

Suppose we have a K-class classifier M, a training set (X_{train}, Y_{train}) and a test set (X_{test}, Y_{test}); a sample is (x_{train}, y_{train}), $y_{train} \in \{1,\ldots,K\}$. After training, we have $M(x_{test})=m=(m_1,m_2,\ldots,m_K)$, $\hat{y}_{test}=argmax(m)$.

Some terms you need to know:

- **Non-Conformity Score**
- **Prediction Set**
- **Coverage: Marginal vs Conditional, Coverage Guarantees**
- **. . .**

1. Conformal Prediction: Vocabulary

Suppose we have a K-class classifier M, a training set (X_{train}, Y_{train}) and a test set (X_{test}, Y_{test}); a sample is (x_{train}, y_{train}), $y_{train} \in \{1,\ldots,K\}$. After training, we have $M(x_{test})=m=(m_1,m_2,\ldots,m_K)$, $\hat{y}_{test}=argmax(m)$.

Goal Today:

Non-Conformity Score: How uncertain is the model about x_{test} belonging to class k? The simplest answer is $S_k=1-c_k$.

Prediction Set: A subset of {1,...,K}: $C=\{1\}$, $C=\{1,\ldots,K\}$, $C=\emptyset$, ...

Coverage: Probability that the true category y_{test} is in $C(x_{test})$.

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3. A Simple Algorithm for Conformal Prediction

Given a Score, how do we build Prediction Sets that have a user-specified coverage?

Given $S=(1-c_1, 1-c_2, \ldots, 1-c_K)$, select a **threshold** t, return c_k if $s_k \leq t$.

How do we choose t ?

Answer: Build a separate dataset (X_{val}, Y_{val}). Ask yourself what level of coverage you want. Find t s.t. you get that level. Use that threshold to build prediction sets on the test set.

3. A Simple Algorithm for Conformal Prediction

Let us build a MWE. We have a 3-category classification task, a trained classifier, a validation set, and we want 80% coverage.

$$\mathcal{M}\left(x_{val}^{1}\right) = (0, 0, 1)$$

$$\mathcal{M}\left(x_{val}^{2}\right) = (0.1, 0.2, 0.7)$$

$$\mathcal{M}\left(x_{val}^{3}\right) = (0.2, 0.3, 0.5)$$

$$\mathcal{M}\left(x_{val}^{4}\right) = (0.4, 0.4, 0.2)$$

$$\mathcal{M}\left(x_{val}^{5}\right) = (0.7, 0.3, 0)$$

$$y_1 = y_2 = y_3 = y_4 = y_5 = 3$$

3. A Simple Algorithm for Conformal Prediction

Let us build a MWE. We have a 3-category classification task, a trained classifier, a validation set, and we want 80% coverage.

$$\mathcal{M}\left(x_{val}^{1}\right) = (0, 0, 1) \Rightarrow S_1 = 0$$

$$\mathcal{M}\left(x_{val}^{2}\right) = (0.1, 0.2, 0.7) \Rightarrow S_2 = 0.3$$

$$\mathcal{M}\left(x_{val}^{3}\right) = (0.2, 0.3, 0.5) \Rightarrow S_3 = 0.5$$

$$\mathcal{M}\left(x_{val}^{4}\right) = (0.4, 0.4, 0.2) \Rightarrow S_4 = 0.8$$

$$\mathcal{M}\left(x_{val}^{5}\right) = (0.7, 0.3, 0) \Rightarrow S_5 = 1$$

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$$y_1 = y_2 = y_3 = y_4 = y_5 = 3$$

Find value q that splits $\{S_i\}$ into 80% below, 20% above. Another name for this is 0.80 quantile.

Return a class k when $1\text{-}c_k < q_{80}$, then you will return 80% of the times the correct class.

3. A Simple Algorithm for Conformal Prediction

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Find value q that splits $\{S_i\}$ into 80% below, 20% above. Another name for this is 0.80 quantile.

Return a class k when $1-c_k<q_{80}$, then you will return 80% of the times the correct class.

$$q_{80} = 0.9$$

0 0.3 0.5 0.8 1

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3. A Simple Algorithm for Conformal Prediction

Let us build a MWE. We have a 3-category classification task, a trained classifier, a validation set, and we want 80% coverage.

$$\mathcal{M}\left(x_{val}^{1}\right) = (0, 0, \underbrace{1}_{>0.1}) \Rightarrow S_1 = 0 \Rightarrow C\left(x_1\right) = \{3\}$$

$$\mathcal{M}\left(x_{val}^{2}\right) = (0.1, \underbrace{0.2}_{>0.1}, \underbrace{0.7}_{>0.1}) \Rightarrow S_2 = 0.3 \Rightarrow C\left(x_2\right) = \{2, 3\}$$

$$\mathcal{M}\left(x_{val}^{3}\right) = (\underbrace{0.2}_{>0.1}, \underbrace{0.3}_{>0.1}, \underbrace{0.5}_{>0.1}) \Rightarrow S_3 = 0.5 \Rightarrow C\left(x_3\right) = \{1, 2, 3\}$$

$$\mathcal{M}\left(x_{val}^{4}\right) = (\underbrace{0.4}_{>0.1}, \underbrace{0.4}_{>0.1}, \underbrace{0.2}_{>0.1}) \Rightarrow S_4 = 0.8 \Rightarrow C\left(x_4\right) = \{1, 2, 3\}$$

$$\mathcal{M}\left(x_{val}^{5}\right) = (\underbrace{0.7}_{>0.1}, \underbrace{0.3}_{>0.1}, 0) \Rightarrow S_5 = 1 \Rightarrow C\left(x_5\right) = \{1, 2\}$$

$$y_1 = y_2 = y_3 = y_4 = y_5 = 3$$

$\boxed{\textbf{Return a class k when } 1\text{-}c_k<0.9}$

4. Concluding Remarks and Further Study

Left out lots of details! For example, if we choose $q_{1-\alpha}$, then we have theoretical guarantees that, if the test set is exchangeable:

$$1-\alpha \leq \mathbb{P}\left(y_{\text{test}} \in C\left(x_{\text{test}}\right)\right) \leq 1-\alpha+\frac{1}{1+n_{\text{val}}}$$

This was the tip of the iceberg, there are extensions for almost every possible machine learning task, some better, some worse.

Conformal Prediction is a distribution-free family of simple and cheap techniques with theoretical guarantees, what's not to love?

4. Concluding Remarks and Further Study

To me, the two most accessible sources of study are:

A. Angelopoulos & S. Bates, *A Gentle Introduction to CP* (see also YT)

C. Molnar, *Introduction to Conformal Prediction with Python*

The UNSURE workshop is starting to publish quite
a bit "conformal papers”, see next slide for a sample.

Also, see our **github** for slides & notebooks!

github.com/agaldran/uqinmia-miccai-2023/tree/main/2024

4. Concluding Remarks and Further Study

- *Y. Zhang et al., RR-CP: Reliable-Region-Based Conformal Prediction for Trustworthy Medical Image Classification, UNSURE 2023*
- *H. A. Mehrtens et al.Pitfalls of Conformal Predictions for Medical Image Classification, UNSURE 2023*

- *C. Clark et al., Conformal Prediction and Monte Carlo Inference for Addressing Uncertainty in Cervical Cancer Screening, UNSURE 2024*
- *A. Wundram et al., Conformal Performance Range Prediction for Segmentation Output Quality Control, UNSURE 2024*
- *G. Ghoshal et al., Making Deep Learning Models Clinically Useful - Improving Diagnostic Confidence in Inherited Retinal Disease with Conformal Prediction, UNSURE 2024*

The END

Thanks!