Master Thesis

Uncertainty Calibration with Online Conformal Prediction in Neural Architecture Search: An Evaluation under the BANANAS Framework

Cheng Chen
(matriculation number 1662473)

July 31, 2025

Submitted to
Data and Web Science Group
Prof. Dr. Margret Keuper
University of Mannheim

Abstract

Some contents

Contents

List of Algorithms

List of Figures

List of Tables

1. Introduction

1.1. Motivation

1.2. Related Work

1.3. Contributions and Limitations

1.4. Outline

2. Literature Review

2.1. Neural Architecture Search (NAS)

2.1.1. Background

NAS is a subfield of AutoML.

Search Space Details will be introduced in 4

Search Strategy

Performance Evaluation

2.1.2. BANANAS

Bayesian Optimization with Neural Architectures for Neural Architecture Search (BANANAS)

BANANAS is an Bayesian Optimization based search strategy.

Bayesian optimization is a sequential decision-making process that seeks to find a global minimum x argminxX f(x) of an unknown black-box objective function f : X R over an input space X RD.

Give an introduction how Bayesian Optimization works. We list the five engineering decisions and review each field's related works. Maybe briefly cite Gaussian Process.

Architecture Encoding

Neural Predictor

Uncertainty Calibration

Acquisition Function

Acquisition Optimization

2.2. Uncertainty Quantification

Understanding uncertainty is important for real-world application of artificial intelligence, e.g., in autonomous driving, medical diagnosis.

2.2.1. Types of Uncertainty

- aleatory uncertainty (data uncertainty): uncertainty that arises due to inherent variations and randomness, and cannot be reduced by collecting more information
- epistemic uncertainty (model uncertainty): uncertainty that arises due to lack of knowledge, and can be reduced by collecting more information.

2.2.2. Alternative Uncertainty Estimation Methods

- Bayesian-based: e.g., Bayesian Neural Network
- Ensemble-based: e.g., Monte-Carlo dropout
- Bootstrapping

But these techniques are limited in several perspectives. First, quantifying uncertainty requires training models for several times, which means that the models cannot be applied for real-time prediction or in an online-learning setup. Second, some models are pre-trained and are only accessible via API. Besides, models (pre-)trained on certain datasets may struggle to generalize across different domains or contexts.

2.3. Conformal Prediction

2.3.1. Theoretical Background

Starting from i.i.d data, and provide an intuitive demonstration how the prediction interval is constructed (can add a figure illustrating why conformal prediction works, i.e., symmetry). From the most intuitive expression to the finite-sample adjusted expression.

Terminology Then, relax the i.i.d assumption to exchangeability, and lay a formal definition of the conformal prediction. And list the most importance three ingredients of the conformal predictions.
- A trained predictor f
- A conformity score function s. The conformity score is an important engineering decision and has an impact on the size on the prediction set, i.e., the efficiency. The conformity score function can be either a negatively- or positively oriented, in which … And it can be a random variable as well.
- A target coverage alpha

Marginal coverage is guaranteed regardless of the choices in dataset and black box model. Only the model predictions are required to apply the technique.

A Link to Statistical Testing (clarify the relationship between conformal prediction and hypothesis testing) In this video (22:21), it is explained the intuition why conformal prediction guarantees the coverage, which is quite similar to the spirit of hypothesis testing.

The coverage parameters which should be pre-set plays a similar role as the confidence interval in hypothesis testing. Conformal prediction is like hypothesis testing with hypotheses:

Table 2.1.: Comparison between CP and Hypothesis Testing

CP	**Hypothesis Testing**
(desired) Coverage level	Confidence level
Nominal error level (1 - Coverage level)	Significance level
The conformity score of the new instance	p-value (is an empirical term)

H0: test instance i conforms to the training instances.
H1: test instance i does not conform to the training instances.

2.3.2. Online Conformal Prediction

2.3.3. Limitations and Extensions

Limitations of split conformal predictions: - Distribution shift. The conformal prediction is built on the core assumption of exchangeability, which means the data points are identically distributed. However, this assumption is hard to meet in real-world application. For example, with time-series data this assumption is generally violated due to the temporal relationships. - Adaptivity. Once the conformity scores are computed on the calibration set, the decision threshold is settled and is applied to all test datapoints, regardless of the intrinsic complexity of the exact example. It is desirable that the threshold can adapts to the difficulty of the problem and produce a larger prediction interval/set on hard-to-solve example and smaller prediction interval/set on easy-to-solve example. This limitation echoes with the characteristic of Conformal Prediction that the guaranteed coverage is only marginal over all datapoints but not conditional on a specific data points..

Variations of Conformal predictions have been proposed to overcome the limitations. There are three main streams: - find an empirical coverage rate which leads to the desired coverage level. For example, if the desired coverage rate is 90- find an efficient conformity score: Alternatively, [...] apply the conformal prediction in an online setting to dynamically incorporate the conformity score of new data points. - find suitable predictor: The trained predictor can be just a poor approximation of the real data generation process. Cross-validation / Jackknife +, Conformal Quantile Prediction

Besides, [...] proposes a CP algorithm that samples datapoints using Monte-Carlo sampling to approach the real distribution of labels in case the ground-truth is ambiguous and consequently cause a biased distribution in manually-annotated labels.

3. Methodology

To address the limitations of the Gaussian assumption in uncertainty estimation, this work introduces a new framework that integrates conformal prediction-based uncertainty calibration into the BANANAS framework in an online setting. An algorithm outlining the overall procedure is presented in Section 3.1, followed by detailed descriptions of each methodological step. Section 3.2 presents different conformal predictions algorithms to be explored. Next, methods for the estimation and evaluation of the conditional distribution of each candidate architecture are discussed in Section 3.3. Finally, in Section 3.4 we introduce how the calibrated distribution can be combined with different acquisition functions and acquisition search strategies.

3.1. The BANANAS–CP Framework

Refer to Section 2.1.2 for a detailed introduction of the original BANANAS algorithm. In this section, we emphasis the key ideas of the uncertainty calibration mechanism, as outlined in Step 1 to 6 of the inner iteration in Algorithm 1.

Bayesian optimization is a form of sequential decision-making task. In the applications of neural architecture search, the typical goal is to find the architecture that has the best evaluation performance on a fixed dataset under a given search budget. At each ietration t, a surrogate model is trained on all architectures evaluated at step $\{0, 1, 2..., t-1\}$, to predict the validation accuracy $f(a)$ of unseen architectures for the next search.

In the standard BANANAS setting, the surrogate model is an ensemble of m feed-forward neural networks, typically $m = 5$. At iteration t, a set of candidate architectures is sampled, and a conditional Gaussian distribution is estimated for each candidate based on the ensemble predictions, as expressed below:

$$\hat{f}(a) \sim \mathcal{N}\left(\frac{1}{m}\sum_{i=1}^{m} f_i(a),\ \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(f_i(a) - \frac{1}{m}\sum_{j=1}^{m} f_j(a)\right)^2}\right) \tag{3.1}$$

where a denotes an architecture sampled from the search space, and $f_i(a)$ is the prediction of the i-th ensemble model for architecture a.

In the BANANAS–CP framework, a key distinction is that all previously evaluated architectures are split into a training set and a calibration set. Then, the surrogate model is trained exclusively using samples in the training set, while the calibration set is used to compute conformity scores for quantile calibration. In practice, at each iteration t, the surrogate model estimates a distribution $\hat{F}$ for an unseen architecture

Algorithm 1 The BANANAS–CP Framework

Input - NAS parameters: search space $\mathcal{A}$, evaluation dataset $\mathcal{D}$, exploration budget T, the number of initially sampled architectures t_0, acquisition function ϕ, surrogate model $\mathcal{M}$ that approximates the true objective function, function $f(\cdot)$ returning validation error of an architecture after training.

Input - Calibration parameters: a function $C(\cdot)$ to create calibration set, a conformity score function $s(\cdot)$, and an array of desired quantile levels q.

Draw t_0 architectures $\{a_0, a_1, ..., a_{t_0}\}$ uniformly at random from $\mathcal{A}$ and train each individual architecture on $\mathcal{D}$.

$\mathcal{A}_{t_0} \leftarrow \{a_0, a_1, ..., a_{t_0}\}$,

for t in $t_0, ..., T$ **do**

1. Apply $C(\cdot)$ and split the trained t_0 architectures into two disjoint datasets; use them as a training set $\mathcal{A}_{t,train}$, and a calibration set $\mathcal{A}_{t,cal}$.
2. Train the surrogate model $\mathcal{M}$ on $\{a, f(a)\}, a \in \mathcal{A}_{t,train}$ using the path encoding to represent each architecture.
3. Compute the conformity scores s on $\mathcal{A}_{t,cal}$.
4. Generate a set of candidate architectures from $\mathcal{A}$.
5. **for** each a_i in candidates **do**
   a) Estimate the quantile value for each level in q and calibrate with conformity scores computed in the previous step.
   b) Fit a distribution F_i based on the estimated quantile values.
   c) Compute the acquisition score $\phi(a_i)$.
6. **end for**
7. Denote a_{t+1} as the candidate architecture with maximum $\phi(a)$; evaluate $f(a_{t+1})$.
8. $\mathcal{A}_{t+1} \leftarrow \mathcal{A}_t \cup \{a_{t+1}\}$

end for

Output: $a^* = \text{argmin}_{t=0,...,T} f(a_t)$

over its validation accuracy on the target dataset, typically either based on a specific distribution assumption or a probabilistic modeling approach, e.g., Bayesian Neural Network. Following the definition in [1], calibration means that for any quantile level $p \in [0, 1]$, the empirical fraction of data-points below the p-th percentile of the predicted distribution $\hat{F}$ should converge to p as the sample size goes to infinity. For example, if p = 80%, then the 80th percentile of $\hat{F}$ is set to the threshold value such that 80% of previously evaluated architectures fall below, thereby aligning with the empirical coverage. In an online setting, the objective of the calibration process can be defined as:

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{I}\left\{y_t \leq Q_t(p)\right\} \rightarrow p \quad \text{for all } p \in [0, 1] \tag{3.2}$$

as $t \rightarrow \infty$, where $\mathbb{I}$ is the indicator function and $Q_t(p)$ represents the distribution $\hat{F}$ in the format of quantile function.

Next, as in the standard Bayesian optimization process, the acquisition function picks the architecture for the next evaluation based on the conditional distribution of all sampled candidates.

3.2. Uncertainty Calibration Algorithms

As reviewed in 2.3, numerous conformal prediction algorithms have been proposed in recent research. This work identifies several approaches applicable in NAS for dividing a dataset into a training set and a calibration set. This section provides an overview of these splitting strategies, as well as the conformity scoring functions that are commonly used for regression problems.

3.2.1. Split Conformal Prediction

To begin, a natural choice for a baseline strategy is the Split Conformal Prediction (SCP).

3.2.2. Cross Conformal Prediction

Conformal Prediction with Cross-validation / Jackknife+

3.2.3. Conformal Prediction with Bootstrapping

3.3. Distribution Estimation

with ensemble, with quantile regressor.

3.4. Acquisition Function and Search Strategy

....

4. Dataset

We run experiments of both algorithms on the widely used benchmark dataset NAS-Bench-201, and compare the performance of BANANAS + CP to the original BANANAS algorithms to assess the role of uncertainty calibration.

5. Experiments and Results

5.1. Setup

6. Conclusion

This chapter presents the central findings of this work as well as their critical discussion. Finally, it highlights limitations and corresponding opportunities for further research.

Bibliography

[1] Shachi Deshpande, Charles Marx, and Volodymyr Kuleshov. Online calibrated and conformal prediction improves bayesian optimization. In *Proceedings of the 27th International Conference on Artificial Intelligence and Statistics (AISTATS)*, volume 238, pages 7262–7273. PMLR, 2024.

A. Additional Experimental Results

Ehrenwörtliche Erklärung

Ich versichere, dass ich die beiliegende Bachelor-, Master-, Seminar-, oder Projektarbeit ohne Hilfe Dritter und ohne Benutzung anderer als der angegebenen Quellen und in der untenstehenden Tabelle angegebenen Hilfsmittel angefertigt und die den benutzten Quellen wörtlich oder inhaltlich entnommenen Stellen als solche kenntlich gemacht habe. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen. Ich bin mir bewusst, dass eine falsche Erklärung rechtliche Folgen haben wird.

Declaration of Used AI Tools

Tool	Purpose	Where?	Useful?
ChatGPT	Rephrasing	Throughout	+

Unterschrift
Mannheim, den 31.07.2025