Master Thesis

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

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July 31, 2025

Submitted to
Data and Web Science Group
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Abstract

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1. Introduction

BANANAS with Conformal Prediction (BANANAS-CP)
Bayesian Optimization with Neural Architectures for Neural Architecture Search (BANANAS)
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1.1. Motivation

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1.4. Outline

Having gained an overview of the research question and the background, the remainder of this thesis is organized as follows. First, Chapter 2 reviews the related works on neural architecture search, uncertainty quantification, and in particular, conformal prediction. In Chapter 3, after proposing a novel framework to incorporate uncertainty calibration into the architecture search process in Section 3.1, we describe its methodological steps in more detail. In Section 3.2, we identify different types of conformal prediction algorithms that are applicable for NAS, and consider the use of the underlying surrogate models. In Section 3.3 and Section 3.4, we further examine how the calibrated predictions can be applied in a Bayesian optimization process. In Chapter 4, we describe the benchmark dataset used for conducting experiments and comparing algorithm performance against the state-of-the-art techniques. In Chapter 5, we present the experiment setups and provide interpretations of the results. Finally, Chapter 6 and Chapter 7 conclude this work and discuss potential future directions.

2. Background

This chapter offers the technical background related to the research question of this work. We start by providing a comprehensive overview of NAS and introduce the three dimensions that characterize a NAS algorithm, followed by an anatomy of the high-performing search algorithm BANANAS. Then, we review the existing uncertainty quantification techniques, with a focus on CP algorithms, particularly those related to the novel framework we propose in Chapter 3.

2.1. Neural Architecture Search

2.1.1. Overview

In the recent decades, deep learning has achieved remarkable success in a variety of areas, including computer vision, natural language understanding, and machine translation. This success is partly attributed to the meticulously hand-crafted neural network architectures. With the rising demand for efficient architecture engineering in complex domains, NAS has emerged as a technique for automating the design of neural architectures for specific tasks.

NAS has been a rapidly progressing research domain in the past years. Since the seminal work that achieves competitive performance on CIFAR-10 [39], numerous NAS algorithms built on different techniques have been proposed. In general, NAS algorithms can be characterized by three key dimensions: search space, search strategy, and performance evaluation strategy [11, 34, 35]. Figure 2.1 illustrates a typical architetcture search process.

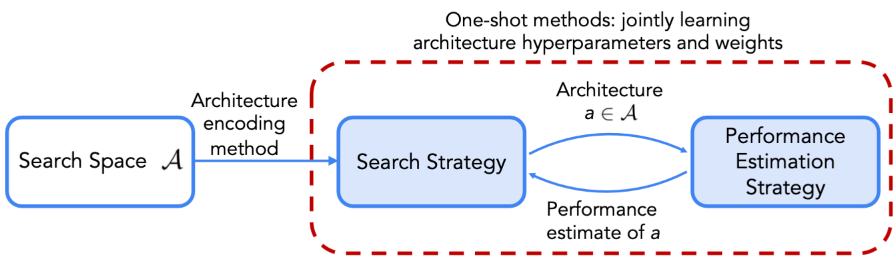


Figure 2.1: Overview of an architecture search process. The search strategy iteratively selects architectures from a predefined search space $\mathcal{A}$. The performance estimation strategy evaluates the model performance on the target dataset and returns the performance to the search strategy.

Next, we provide definitions of the terms and review the research progress of each domain.

Search Space A search space defines a set of architectures that the search algorithm is allowed to select. The search space is often the first step when setting up NAS and perhaps is also the most essential step, because the design of the search space represents an important trade-off between human bias and efficiency of search: a smaller search space incorporating more prior human knowledge and involving more manual decisions will enable NAS algorithms to find high-performing architectures more easily, in contrast a larger space with more primitive building blocks provides higher odds of discovering truly novel architectures [34]. Common search spaces range in size from a few thousand to over 10^{20}.

There are four major categories of search spaces in the NAS literature [34]. We start with two types of search spaces that have relatively simple architecture topologies. The macro search spaces [2, 13, 39] encode the entire neural architecture at a high level. Typically, an entire architecture is often represented by a Directed Acyclic Graph (DAG), with nodes defining the operation types and edges representing data flows. Each node is allowed to have distinct structures, such as convolution, pooling. As a result, macro search spaces are highly flexible and possess high representation power. Another type is the chain-structured search spaces. As suggested by the name, chain-structured search spaces consist of neural networks that can be written as a sequence of operation layers. These search spaces often take state-of-the-art manual designs as the backbone. For example, there are several chain-structured search spaces based on the convolutional networks [7] or the transformer architectures [37].

The third group is the cell-based search spaces, which perhaps are the most popular type of search spaces in NAS research. The cell-based search spaces are inspired by the fact that state-of-the-art human-designed architectures often consist of repeated blocks. For instance, the high-performing Transformer [30] contains 6 identical stacked encoder and decoder layers. Thus, instead of searching for the entire network architecture from scratch, [40] propose to only search over relatively small cells, and stack the cells according to a predefined skeleton to form the overall architecture. Building on this idea, [40] proposes the first modern cell-based search space, NASNet, which comprises of two types of cells: the normal cell that preserves the dimensionality and the reduction cell that reduces the spatial dimension, as illustrated in Figure 2.2. Since its emergence, many other cell-based search spaces have been developed. In general, these cell search spaces share a high-level similarity, but differ in the design of the fixed macro structure, the layout and constraints in the cells, and the choices of operations within the cells [10, 19, 38]. The cell-based approach significantly reduces the size and the complexity of the search space. However, it has been criticized for limiting the expressiveness of NAS, potentially hindering the discovery of highly novel architectures [34].

The last main category is the hierarchical search spaces. Different from the aforementioned types of search spaces that mostly have a flat representation, hierarchical search spaces involve designing patterns at different levels, where each higher-level pattern is often represented as a DAG of lower-level patterns [8, 18].

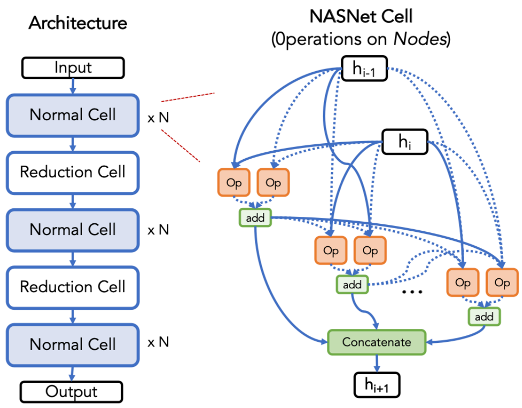


Figure 2.2: Overview of a cell-based search space NasNet. The outer skeleton across cells (left) is fixed, and the operations, represented by nodes, within the cells are searchable (right) [34].

In addition to the architecture topology, another important design accompanying a search space is the architecture encodings, because many NAS algorithms require representations of the architectures to, for example, mutate an architecture or train a predictive model to extrapolate its performance. For search spaces that can be represented by a DAG, adjacency matrix is a commonly used encoding method. In addition, other encoding techniques, including graph-based encoding [24], path-based encoding [33] and conditionally-structured encoding methods tailored for hierarchical search spaces have been proposed. [32] has shown that the effect of the encoding methods varies across different NAS subroutines.

Search Strategy According to [34], there are generally two main categories of search strategies: black-box optimization based techniques and one-shot techniques.

The black-box optimization based techniques largely overlap with another sub-area of AutoML: the hyperparameter tuning. Common techniques for hyperparameter tuning have been proven to be efficient for NAS as well, including reinforcement learning [39, 40], evolutionary algorithms [21, 26], gradient descent[19], and etc. In particular, we take a close look at the search strategies based on Bayesian optimization, since they are closely related to the research question of this work. Specifically, initial Bayesian optimization based approaches typically use the Gaussian Process (GP) as the surrogate model [13]. However, these algorithms often demonstrate under-performance compared to their competitors due to several limitations: 1) search spaces are usually high-dimensional, non-continuous, and graph-like; 2) GPs requires custom distance metrics among architectures, which involves a time-consuming matrix inversion step. Besides, GPs are difficult to scale since the computation complexity grows cubically with the number of observations. To address these challenges, a new framework that using a neural predictor as the surrogate model for Bayesian optimization has been proposed and demonstrated strong performance [20, 29, 33]. We review this framework in details in Section 2.1.2.

The one-shot techniques are introduced to avoid training each architecture from scratch, The key idea is to train a *supernetwork* that comprises all possible architectures in the search space as subnetworks. Once a supernet is trained, each architecture from the search space can be evaluated by inheriting the weights from the corresponding subnet within the supernet [4, 19].

Performance Evaluation The performance evaluation refers to the process of estimating the performance of architectures. The estimated performance is communicated back to the search algorithm to guide the next search. The simplest performance estimation strategy is to fully train an architecture on the training data and then evaluate its performance on the validation data. However, training each architecture demands substantial computation resources and typically takes serval hours or days on a GPU. Consequently, many methods for speeding up the performance evaluation process for architectures have been proposed. One popular line of work is to predict the performance of neural networks before they are fully trained using the zero-cost proxies [22].

In this work, we primarily run experiments on the benchmark dataset NAS-Bench-201 [10], which offers queryable validation and test accuracies for all architectures in the search space and thereby eliminates the need to train neural networks when simulating NAS experiments. Hence, we provide only a brief overview of this aspect and refer the readers to [34] for a comprehensive introduction to the performance evaluation techniques.

2.1.2. Bayesian Optimization and BANANAS

As briefly mentioned in Section 2.1.1, the Bayesian optimization based NAS search strategy using a neural network as the surrogate model has shown strong performance. In particular, after identifying five components of this framework, [33] performs a thorough analysis on each component's effect towards the search performance and proposes a final algorithm, i.e., BANANAS, based on both theoretical and empirical findings. This method is proven to be efficient, achieving state-of-the-art performance on popular NAS benchmarks

In this section, we present a detailed review of the work by [33]. We start with the theoretical background and give an introduction into the Bayesian optimization method. Next, we walk through the five identified components and provide a summary of the experimental findings.

Bayesian optimization [23] is a sequential decision-making process that seeks to find the global maximum (minimum is the negation of the maximum) of an unknown black-box objective function $f : X \rightarrow R$ over an input space $X \subseteq R^D$. In a Bayesian optimization process, the unknown objective function f is treated as a random function and the prior belief over f is encoded by a surrogate model, usually a Gaussian Process or a Parzen-Tree Estimator [5]. At each iteration, the surrogate model updates the prior with the observations and forms a posterior probabilistic distribution of f. Then, the acquisition function, another key component that trades off exploration and exploitation in the process, evaluates a set of candidates based on the posterior distribution and picks

Algorithm 1 Bayesian Optimization

Input: surrogate model $\mathcal{M}$, acquisition function ϕ, objective function $f(\cdot)$, number of iterations T.

1: Initialize the set of observations: $D \leftarrow \emptyset$

2: **for** t in $1, ..., T$ **do**

1. Fit surrogate model $\mathcal{M}$ to current observations set $\mathcal{D}_{t-1}$.
2. Evaluate acquisition function and select the next point for query: $x_t = \text{argmax}_{x \in \mathcal{X}}\ \phi(x,\ \mathcal{M})$
3. Query the objective function: $y_t = f(x_t)$

4. Update the observations set: $\mathrm{D}_t \leftarrow \mathcal{D}_{t-1} \cup \{(x_t, y_t)\}$

3: **end for**

4: **Output:** $x^* = \text{argmax}_{t=1,...,T}\, f(x_t)$

the data point with the largest acquisition score for next query. Algorithm 1 outlines this procedure.

The acquisition function adopted in the original paper [23] is the Expected Improvements (EI). Other popular alternative options include: Thompson Sampling (TS), Independent Thompson Sampling (ITS), Upper Confident Bound (UCB), and Probability of Improvements (PI). Different acquisition functions typically favor exploration and exploitation differently. Nevertheless, [1] shows that EI is competitive in reaching the optimum value with comparably few iterations.

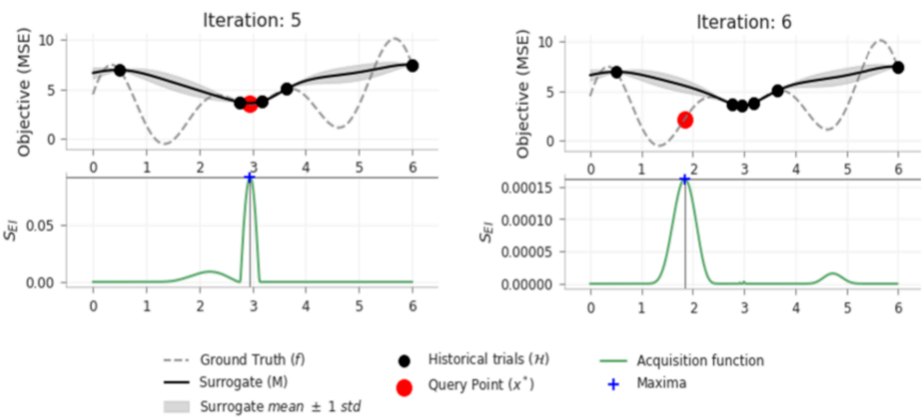


Figure 2.3: Example of Bayesian optimization with Gaussian Process as the surrogate and EI as the acquisition function to explore the minimum of the objective function [1].

Now, we return to the "Bayesian optimization + neural predictor" NAS framework. It becomes obvious that this framework is essentially an optimization task searching the maximum with a neural network as the surrogate and neural architectures in a search space being the inputs. Specifically, [33] identifies five critical components within the framework, which are listed as follows:

Architecture Encoding

Neural Predictor A set of neural architectures and their corresponding validation accuracies are randomly sampled from the search space for training and comparing different neural predictors. Among all neural predictors, including VAEs, GCNs, and FNNs with either the adjacency matrix or path-based encoding, FNNs with path encoding demonstrates the strongest performance.

Uncertainty Estimation Uncertainty estimates are required to form the probabilistic distribution. For Bayesian neural networks (BNNs), the posterior distribution is inferred over the nework weights. For an ensemble of Feedforward Neural Networks (FNNs), the distribution is inferred under the Gaussian assumption. The results show that an ensemble of even only 3 to 5 neural networks in general yields more reliable uncertainty estimates than BNNs.

Acquisition Function In the experiments, five commonly used acquisition functions are examined: TS, ITS, UCB, PI, and EI. Each function is adapted to the Gaussian assumption, thereby requiring only the mean and standard deviation estimates to compute the acquisition scores. In the experiments, overall ITS yields the best performance among all the options, although the marginal outperformance is subtle. The results indicate that the acquisition function does not have as significant impact on the search performance as the other examined components in the framework.

Acquisition Optimization In each iteration of the Bayesian optimization, the goal is to select a candidate from the search space that maximizes the acquisition score. Evaluating the acquisition function for every architecture available in the search space is computationally infeasible, therefore [33] proposes to create a set of 100 to 1000 candidates and then choose the architecture with the maximal acquisition score in this set. Specifically, [33] explores various approaches for creating this candidate set. The simplest and most natural way is to draw architectures at random. Consider that architectures close in edit distance to those used for training the surrogate model are likely to have more accurate estimates, an alternative is a mutation-based sampling approach, where the candidate set is created via local search by randomly modifying an operation or an edge of the best-performing architectures that have been evaluated so far. In additional, [33] also examines a hybrid approach that combines random search with mutation-based search. Their experiments show that the mutation-based approach outperforms its competitors and suggest it is better to search locally rather than globally.

Finally, the best components found in the aforementioned analyses are transformed into the BANANAS algorithm, which composed of an ensemble of FNNs using the path encoding, and ITS with a mutation strategy for acquisition (Figure 2.4).

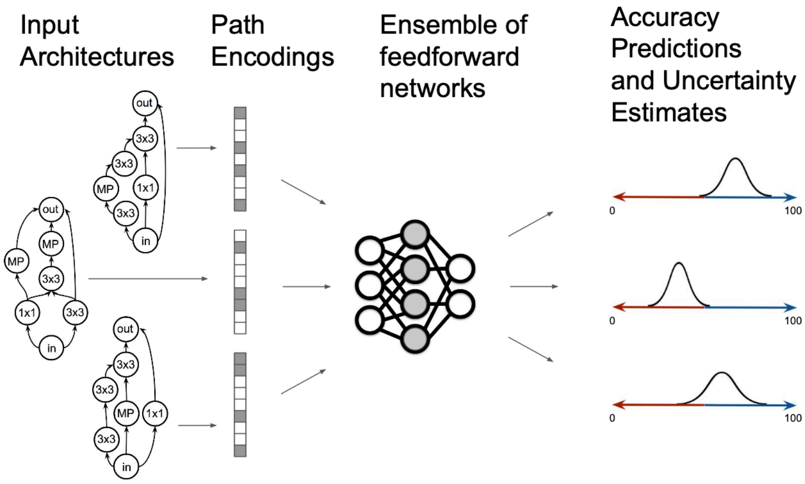


Figure 2.4: Diagram of the BANANAS framework.

2.2. Uncertainty Quantification Methods

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

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.

- 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. uncertainty calibration using another regressor.

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.

Notation 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.

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)

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

2.3.2. Full Conformal Prediction

Full Conformal Prediction (FCP)

2.3.3. Extensions of Conformal Prediction

Since the transductive version of CP was first proposed in [12], several variants have been developed with different computational complexities, formal guarantees, and practical applications.

To address the aforementioned inefficient computation problem of FCP, Split Conformal Prediction (SCP), also known as Inductive Conformal Prediction (ICP), was first introduced in [25] by replacing the transductive inference with inductive inference. aims to learn a general prediction rule about the data using the observed records. Then, this rule can be applied directly to obtain predictions when new data arrives in sequence, without re-using the training data and retraining the model repeatedly. The main concept involves splitting the data into two non-overlapping subsets, designated for training and calibration, respectively. A predictive model is fit exclusively on the training set, then non-conformity measures are computed on the calibration set to determine the prediction interval's width. Due to its simplicity and computational efficiency, SCP is one of the most commonly used techniques in the CP family. We delve into methodological steps of SCP with pseudo-code in Section 3.2.1.

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.

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

Despite of its provable strength, BANANAS assumes a Gaussian distribution for measuring uncertainty. However, this assumption does not necessarily hold in real world. To mitigate the potential limitations caused by inaccurate uncertainty estimates, 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 of BANANAS-CP 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 in Section 3.3, methods for the estimation and evaluation of the conditional distribution of each candidate architecture are discussed. Finally, in Section 3.4 we introduce how the calibrated distribution can be combined with different acquisition functions and acquisition search strategies in the Bayesian optimization process.

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 2.

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 $\{0, 1, 2..., t-1\}$ and their associated validation accuracies, to predict the scores 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 predicted accuracy from the i-th base learner of the ensemble for architecture a.

Algorithm 2 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 non-conformity score function $s(\cdot)$, and an array of desired quantile levels q.

Draw t_0 architectures $\{a_1, a_2, ..., a_{t_0}\}$ uniformly at random from $\mathcal{A}$ and train each individual architecture on $\mathcal{D}$.

$\mathcal{A}_{t_0} \leftarrow \{a_1, a_2, ..., a_{t_0}\}$,

for t in $t_0 + 1, ..., T$ **do**

1. Apply $C(\cdot)$ and split all evaluated 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 $\mathcal{M}_t$ 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 value for each quantile level q_i in q and calibrate using conformity scores computed in the previous step, with q_i implying a mis-coverage rate $2q_i$ or $2(1 - q_i)$ for conformal prediction.
   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 as the candidate architecture with maximum $\phi(a)$; evaluate $f(a_t)$.
8. $\mathcal{A}_t \leftarrow \mathcal{A}_{t-1} \cup \{a_t\}$

end for

Output: $a^* = \text{argmax}_{t=1,...,T} f(a_t)$

In the BANANAS-CP framework, a key distinction is that all architectures evaluated at step $\{0, 1, 2..., t-1\}$ are divided disjointly 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 conditional distribution $\hat{F}$ for an unseen architecture over its validation accuracy on the target dataset, either based on a specific distribution assumption or a probabilistically-interpretable modeling approach, e.g. quantile regression. Following the definition in [9, 16], 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:

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

as $t \to \infty$, where $\mathbb{I}$ is the indicator function and $Q_t(p)$ represents the distribution $\hat{F}$ in the format of quantile function [9, 16].

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 Section 2.3, numerous conformal prediction algorithms have been proposed in recent research. This work identifies several approaches applicable in NAS for building a calibration set and computing conformity scores. 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 calibration strategy is the SCP. In this section, we start by introducing the standard SCP procedure, then proceed with the adaptions required to incorporate it into the BANANAS-CP framework.

Implementation steps of SCP are summarized in Algorithm 3. Imagine a regression task where the non-conformity level is measured by the absolute residual, i.e. $|y_i - \hat{y}(x_i)|$. In this case, the algorithm produces a prediction interval for the test point with a width of $[\hat{y}_{test} - \hat{q}\ ,\ \hat{y}_{test} + \hat{q}]$, where $\hat{q}$ is the conformity threshold as defined in line 6.

In this work, we explore SCP in combination with different prediction algorithms. First, we follow the settings in BANANAS and use an ensemble of five FNNs as the

Algorithm 3 Split Conformal Prediction

Input: A set of observations $\{(x_i, y_i)\}_{i=1}^n$, a prediction algorithm $h(\cdot)$, a non-conformity measure $s(\cdot)$, nominal mis-coverage rate τ, fraction of data assigned to the training set p_{train}, test data x_{n+1}.

Output: a prediction set $\mathcal{C}_\tau(x_{n+1})$ that covers y_{n+1} with probability $1 - \tau$.

1: Allocate at random a proportion of p_{train} of the observations to the training set $\mathcal{D}_{train}$ and use the rest for calibration $\mathcal{D}_{cal}$.
2: Train the point predictor $h(\cdot)$ on $\mathcal{D}_{train}$.
3: Initialise a scoring set $S = \emptyset$
4: **for** (x_i, y_i) in $\mathcal{D}_{cal}$ **do**
    $S \leftarrow S \cup \{s(h(x_i), y_i)\}$
5: **end for**
6: Return $\mathcal{C}_\tau(x_{n+1}) \leftarrow \{y \,|\, s((h(x_{n+1}), y) \leq q\}$, where q is the $\lceil(1-\tau)(n_s+1)\rceil$-th smallest value of S, with $n_s = |S|$.

underlying surrogate model. In this case, note that the bounds of the prediction set as identified in Algorithm 3 should not be simply interpreted as the quantile values of a distribution, since the prediction algorithm does not directly model the τ-quantile of the variable Y, i.e., $Q_Y(\tau) = F_Y^{-1}(\tau) = \inf\{y \colon F_Y(y) \geq \tau\}$, with $\tau \in [0,1]$ denoting a quantile level and F_Y its cumulative distribution function. Thus, the ensemble predictor must be used in conjunction with a valid distribution assumption to obtain valid quantile values. Motivated by the goal of achieving a completely distribution-agnostic solution, we next replace the ensemble model with a quantile regressor that directly models the quantiles of a distribution. In the remainder of this section, we discuss the configurations designated for each prediction algorithm.

Ensemble Predictor Following the settings in the original BANANAS, an ensemble by default consists of five neural networks, where each neural network is a fully-connected multi-layer perceptron with 20 layers of width 20. The neural networks are trained by minimizing the mean absolute error (MAE), using the Adam optimizer with a learning rate of 0.01. In parallel to BANANAS, we assume that the validation accuracy of each unseen candidate architecture a follows a Gaussian distribution, which is parameterized by the predictive mean ($\hat{\mu}$) and standard deviation ($\hat{\sigma}$) provided by the ensemble model, as demonstrated in equation 3.1. For a specific significance level α (suppose $\alpha < 0.5$), the central quantile interval can be written as:

$$\left[\hat{\mu} - \Phi^{-1}_{1-\alpha/2} \cdot \hat{\sigma}\ ,\ \hat{\mu} + \Phi^{-1}_{1-\alpha/2} \cdot \hat{\sigma}\right] \tag{3.3}$$

where $\Phi^{-1}_{1-\alpha/2}$ denotes the $(1-\frac{\alpha}{2})$-th quantile of the standard normal distribution.

Now, take a closer look at the formula 3.3 and recall the example based on the absolute residuals, which is presented earlier in this section. We observe that the confidence interval under the Gaussian assumption takes a close form to the prediction interval produced by CP when the conformity scoring function is exactly chosen as:

$$s(\cdot) = \frac{|y_i - \hat{y}(x_i)|}{\hat{\sigma}(x_i)} \tag{3.4}$$

Hence, the bounds of the CP-derived prediction interval can be *approximately* interpreted as empirically calibrated quantile estimates under the Gaussian assumption, provided that the conformity scoring function is chosen appropriately. Note that the absolute residual can be seen as a special case of equation 3.4 as well, where the empirical standard deviation estimate is disregarded and fixed at one. In fact, this scaled absolute residual (equation 3.4) is a popular choice for measuring conformity in practice. Ideally, we would like the CP-derived prediction interval also demonstrates local adaptivity, i.e., the prediction interval should have a larger width if the prediction task is difficult and smaller otherwise. The scaled absolute residual accounts for heteroskedasticity and is able to adjust the width of the prediction band by multiplying the standard deviation estimate. In contrast, the band produced with a pure residual score has constant-width everywhere regardless of the input, which limits its effectiveness in application. Therefore, in this work, we use the scaled absolute residual as the conformity scoring function for ensemble predictors, unless otherwise specified.

Quantile Regressor We now explain how a quantile regressor can be leveraged to build a probabilistic surrogate for Bayesian optimization. We follow the methods established previously in [27, 28].

We start with a brief introduction into the quantile regression [15]. Suppose $(x, y) \sim F$ denote data drawn from a joint distribution that is characterized by its cumulative distribution function F, the aim of the conditional quantile regression is to estimate a given quantile of the conditional distribution of Y given $X = x$. The conditional quantile function for α-quantile is:

$$Q(\alpha) = \inf \{ y \in \mathbb{R} : \mathbb{P}(Y \leq y \mid X) \geq \alpha \} \tag{3.5}$$

and can be estimated by minimizing the Pinball loss on the training data [15]:

$$\ell_\alpha(y, \hat{y}) = \begin{cases} \alpha(y - \hat{y}), & \text{if } y \geq \hat{y} \\ (1-\alpha)(\hat{y} - y), & \text{otherwise} \end{cases} \tag{3.6}$$

where $\hat{y}$ is the predicted quantile value. As illustrated in Figure 3.1, the Pinball loss is asymmetric and the intuition behind is that under-estimate and over-estimate receive different penalties across quantiles. For instance, if $\alpha = 0.9$, then we would expect that empirically 90% of observations should fall below the prediction. In this case, the loss function places a higher penalty for underestimate.

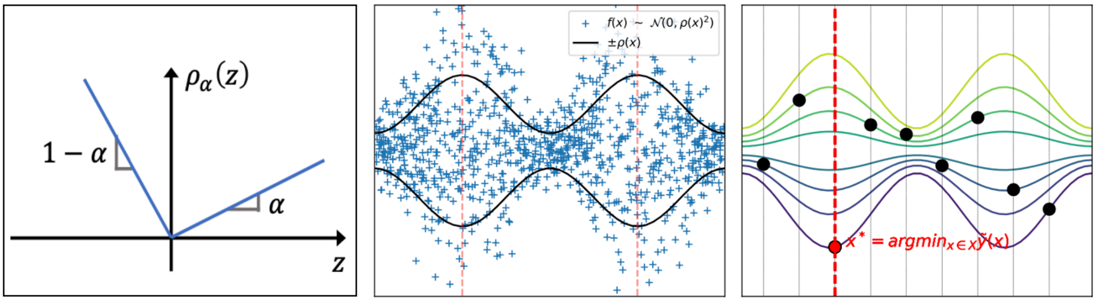


Figure 3.1: Visualization of the Pinball loss function, where $z = y - \hat{y}$ [27] (left); Samples from a synthetic heteroskedasticity function (middle) and the sampling procedure based on $|q| = 8$ predicted quantiles [28] (right).

Quantile regression in the BANANAS-CP framework is implemented by training a dedicated neural network for each quantile level q_i in the array q as defined in Algorithm 2 using the corresponding Pinball loss $\ell_{q_i}(y, \hat{y})$.

While quantile regression can model the shape of any continuous distribution given enough data, the predictions are not guaranteed to be well calibrated in practice. In fact, it is not uncommon that quantile regression generates non-monotonic predictions, a phenomenon referred as quantile crossing. To address this issue, we apply a post-hoc calibration upon the predicted quantiles using the Conformal Quantile Regression (CQR) from [27]. This method consists of a novel conformity score tailored for quantile estimation and the key idea of calibration is to apply quantile-aware offsets, which are computed on the calibration set, on the original predicted quantiles.

A close work is [28] that employs CQR to obtain quantiles with robust coverage during hyperparameter tuning via Bayesian optimization. Specifically, the calibrated quantiles are used to select the candidate for the next search, where a set of candidates is first sampled uniformly at random, and then for each of those candidates a random quantile is simply picked and is treated as the acquisition score (Figure 3.1). We follow their notation and interpretation in defining the conformity score for a quantile surrogate:

$$E_i = \max\left\{\hat{q}_{\alpha_j}(x_i) - y_i,\ y_i - \hat{q}_{1-\alpha_j}(x_i)\right\} \tag{3.7}$$

where $\hat{q}_\alpha(x_i)$ denotes the predicted α-quantile at x_i. Note that the sign of the score is positive when the target y_i is outside of the interval and negative when the target falls inside the predicted interval. This allows the conformity score to account for both overcoverage and undercoverage cases. In addition, the score amplitude always measures the distance to the closer quantile between $\hat{q}_{\alpha_j}(x_i)$ and $\hat{q}_{1-\alpha_j}(x_i)$ [27, 28].

3.2.2. Conformal Prediction with Cross-validation

Solving a NAS problem is usually computationally expensive, as each neural architecture evaluation incurs the cost of fully training and validating the underlying model on the target dataset. Motivated by the fact that NAS based on Bayesian optimization is typically allocated with a budget of 100 to 200 epochs, an additional heuristic for constructing the calibration set via cross-validation (hereafter: CrossVal-CP) is employed to avoid reducing the sample size for obtaining a holdout set as performed in SCP.

The CrossVal-CP method is a natural extension of SCP and is first formally presented in [31]. At each step, the evaluated architectures are devided at random into K folds. A dedicated surrogate model is trained on $K-1$ folds, while the remaining one is used as the calibration set to calculate the conformity scores. This process is repeated for K times over each individual fold. Finally, conformity scores from all calibration folds are combined to form the overall calibration set, on which the quantile is computed to determine the calibration offset. For an unseen data point, the prediction is obtained by aggregating the predictions of the K trained models, e.g., by taking the average of the model outputs. Algorithm 4 summarizes this procedure.

Algorithm 4 Conformal Prediction with Cross-validation

Input: A set of observations $\{(x_i, y_i)\}_{i=1}^n$, number of folds K, a prediction algorithm $h(\cdot)$, a non-conformity measure $s(\cdot)$, nominal mis-coverage rate τ, test data x_{n+1}.
Output: a prediction set $\mathcal{C}_\tau(x_{n+1})$ that covers y_{n+1} with probability $1-\tau$.

1: Initialise a conformity scoring set $S = \emptyset$
2: Split the observations $\{(x_i, y_i)\}_{i=1}^n$ into K folds at random. I_k denotes the index set containing indices of samples in the k-th fold.
3: **for** k in 1, 2, ..., K **do**
   1. Train $\hat{h}_{-k}(\cdot)$ on $\{(x_i, y_i) \mid i \notin I_k\}$
   2. Compute conformity score on the k-th fold $S_k = \{s((\hat{h}_{-k}(x_i), y_i) \mid i \in I_k\}$
   3. $S \leftarrow S \cup S_k$
4: **end for**
5: Predict x_{n+1}: $h(x_{n+1}) \leftarrow aggregate(\{\hat{h}_{-1}(x_{n+1}), ..., \hat{h}_{-K}(x_{n+1})\})$
6: Return $\mathcal{C}_\tau(x_{n+1}) \leftarrow \{y \mid s((h(x_{n+1}), y) \le q\}$, where q is the $\lceil (1-\tau)(n_s+1) \rceil$-th smallest value of S, with $n_s = |S|$.

Note that the only distinction between SCP and CrossVal-CP is how the calibration set is constructed. Since it does not place any additional restriction on the choices of the underlying surrogate, CrossVal-CP can be applied in conjunction with either ensemble predictor or quantile regressor in the same way as SCP. See Section 3.2.1 for detailed configurations.

3.2.3. Conformal Prediction with Bootstrapping

Inspired by the fact that BANANAS is built on an ensemble surrogate, we further explore incorporating Jackknife+-after-boostrap [14], a wrapper for predictive inference

Algorithm 5 Conformal Prediction with Bootstrapping

Input: A set of observations $\{(x_i, y_i)\}_{i=1}^{n}$, number of bootstraps B, a prediction algorithm $h(\cdot)$, a non-conformity measure $s(\cdot)$, nominal mis-coverage rate τ, test data x_{n+1}.

Output: a prediction set $\mathcal{C}_\tau(x_{n+1})$ that covers y_{n+1} with probability $1-\tau$.

Sample all available data with replacement and create B subsets. I_b denotes the indices of data points included in the b-th sample.

Train $\hat{h}_b(\cdot)$ on $\{(x_i, y_i) \mid i \in I_b\}$ for b in 1, 2, ..., B

Initialise a conformity scoring set $S = \emptyset$

for i in 1, 2, ..., n **do**

1. Initialize an empty for leave-one-out estimates $LOO_i = \emptyset$
2. For b in 1, 2, ..., B, if $i \notin \mathrm{I}_b$: $LOO_i \leftarrow LOO_i \cup \hat{h}_b(x_i)$

3. S $\leftarrow S \cup s\big(aggregate(LOO_i),\ y_i\big)$

end for

Predict x_{n+1}: $h(x_{n+1}) \leftarrow aggregate(\{\hat{h}_1(x_{n+1}), ..., \hat{h}_B(x_{n+1})\})$

Return $\mathcal{C}_\tau(x_{n+1}) \leftarrow \{y \,|\, s((h(x_{n+1}), y) \leq q\}$, where q is the $\lceil(1-\tau)(n_s+1)\rceil$-th smallest value of S, with $n_s = |S|$.

designed specifically for use with ensemble learners, into the calibration step (hereafter: Bootstrap-CP).

In contrast to fitting m neural networks on the same training data with different random weights initializations, as applied in the BANANAS framework, a different technique to build an ensemble model is via bootstrapping. Specifically, the ensemble method starts by creating multiple training datasets by resampling the available data points with replacement. In the next step, multiple models are trained on each of the bootstrapped subsets, and their predictions are aggregated to produce the single final prediction [6]. This technique offers more accurate and stable estimates than a single model and has shown superior performance in application.

Jackknife+ is a type of CP algorithm that is closely related to the leave-one-out (LOO) method [3]. Given a set of observations $\{(x_i, y_i)\}_{i=1}^{n}$, the idea is to fit an LOO estimator $\hat{h}_{-i}$ using all available data except for the i-th sample, and this process iterates over all individual samples. Then, the predictive interval around the i-th point is obtained by offsetting the prediction from $\hat{h}_{-i}(x_i)$ with the quantile of all LOO conformity scores. Equivalently, Jackknife+ can be viewed as a special case of CrossVal-CP when the number of folds is exactly set to $K = n$.

Jackknife+-after-boostrap [14] integrates both approaches and provides a cost-efficient wrapper by leveraging only the available bootstrapped sets and their corresponding fitted models, thereby avoiding re-fitting ensembles on each individual bootstrapped sample. [36] extends this method to online setting and proves its efficiency for time-series data. In contrast to the CP algorithms described in earlier sections, Bootstrap-CP requires no data splitting because sampling with replacement automatically creates holdout sets. Training the bootstrap ensemble on random subsets from the full data also reduces the chance of overfitting.

Implementation of Bootstrap-CP is shown in Algorithm 5. Noteably, if a particular data point appears in all bootstrapped samples, it is then excluded from the computation of conformity scores since it has no associated LOO estimator. In Bootstrap-CP, the absolute residual is mainly used for measuring conformity, due to potentially insufficient LOO outputs for standard deviation estimation, i.e., LOO_i in Algorithm 5 might have fewer than two points. Specifically, Bootstrap-CP is only applied with the ensemble model. This concludes our experiment setups and the BANANAS-CP framework is finally evaluated under five various predictor+CP configurations.

3.3. Distribution Estimation

As described in Section 2.1.2, Bayesian optimization generally relies on a continuous posterior distribution at $X = x$ to obtain the acquisition score. Here, we denote by $F_t(x)$ the Cumulative Distribution Function (CDF) of the posterior distribution of the data point x at step t. In the context of NAS, where the target variable is assumed to be continuous and real-valued, the distribution can be represented by the inverse of its CDF, or quantile function without loss of generality, i.e. $Q_t(x) = F_t^{-1}(x)$.

In the BANANAS-CP framework, as outlined in Algorithm 2, we are able to generate calibrated quantile estimates for a finite set of discrete quantile levels. Intuitively, assuming the quantiles estimates are accurate, increasing the granularity of quantile levels should lead to a more accurate approximation of the underlying continuous distribution. However, it is computationally prohibited to estimate an infinite number of quantiles in practice, especially with significantly limited training data. Therefore, we propose an approach for constructing a continuous distribution from discrete quantile estimates with mild assumption. Specifically, the distribution estimator is defined as:

Definition Let $\{q_i\}_{i=1}^n$ be a quantile of percentile levels such that $0 < q_1 < q_2, ..., < q_n < 1$, and $\{v_i\}_{i=1}^n$ are the corresponding quantiles, i.e., $F^{-1}(q_i) = v_i$, the empirical CDF of the distributions $\hat{F}$ is constructed by applying linear interpolation between adjacent quantiles. Consequently, the Probability Density Function (PDF) of a specific interval $(v_a, v_b), a, b \in \{1, ..., n\}$ and $a < b$ is:

$$PDF(x) = \frac{q_b - q_a}{v_b - v_a}, \quad \text{if } x \in (v_a, v_b)$$

Diagnosis Analysis To assess the validity of this approach, we first perform a diagnosis analysis using synthetic datasets generated by a left-skewed Gaussian distribution, which we believe resembles the true underlying distribution of the validation performances of architectures in a search space. The experiments on the synthetic data are intended to reflect the comparisons in a real NAS application, therefore two kinds of distribution estimators are examined: a Gaussian estimator and a linear-interpolation based quantile estimator. The analysis is repeated with different parameterizations, e.g, the number of quantiles, or the size of the samples, etc.

Table 3.1 reports the performance of three distribution estimators on synthetic datasets with various sample sizes. In particular, the linear-interpolation based quantile estimator is evaluated under 10 and 20 quantile levels, and the quantile estimates for interpolation are obtained by taking the empirical quantiles of the sample data. The estimation performance is assessed using the mean, standard deviation and Kullback–Leibler (KL) divergence [17]. For each sample size, we run 50 trials and aggregate the metrics over the trials to reduce the effects of randomness. Results in Table 3.1 indicate that the linear-interpolation based quantile estimator offers a better approximation to an asymmetric distribution than a Normal distribution, and increasing the number of quantile levels leads to improved approximation performance, provided with sufficient data. However, a caveat is that quantile-based estimation tends to produce biased standard deviation estimates, which may lead to undesired effect.

Having considered the behaviors of the various acquisition functions employed in the real BANANAS-CP application (see Section 3.4), we additionally present several visualizations based on a synthetic dataset with 150 samples (Figure 3.2, Figure 3.3) to confirm the shapes of the estimated distributions are not significantly deviated from that of the true underlying distribution, thereby assuring the effectiveness of the acquisition functions.

Evaluation Metrics Within the BANANAS-CP framework, the calibration quality at a specific epoch is measured by the Root Mean Squared Calibration Error (RMSCE) [16]. Suppose $\hat{F}_t^{-1}$ is the CDF of the distribution estimated at the t-th step and y_t is the true value revealed after the estimation, consider a sequence of $\{(\hat{F}_t^{-1}, y_t)\}_{t=1}^{T}$ that represents a neural architecture search process after T epochs, the calibration error at the T-th epoch is defined as:

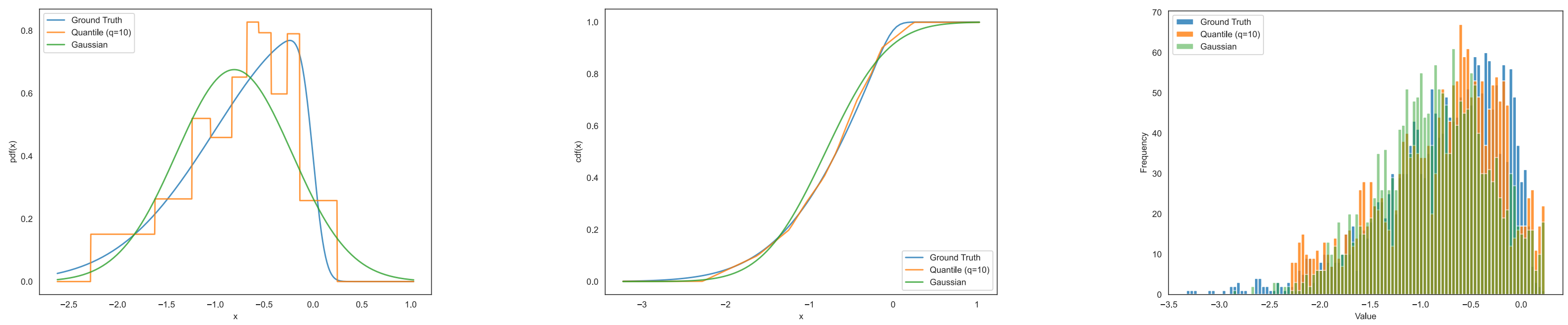
$$\mathrm{RMSCE}\left(\hat{F}_1^{-1}, y_1, \ldots, \hat{F}_T^{-1}, y_T\right) = \sum_{j=1}^{m} w_j \left(p_j - \hat{p}_j\right)^2 \tag{3.8}$$

$$\text{with} \quad \hat{p}_j = \frac{\left|\left\{y_t \;\middle|\; \hat{F}_t^{-1}(y_t) \leq p_j,\ t = 1, 2, \ldots, T\right\}\right|}{T}$$

where m represents the number of discrete quantile levels and the scalars w_j are quantile weights. For simplicity, we adopt $w_j = 1, \forall j \in [0, 1]$ in this work. Alternatively, calibration errors of the quantiles can be weighted by the number of observations falling into the corresponding intervals. Note that calibration errors calculated with different numbers of quantiles are not directly comparable. In general, increasing the number of quantiles tends to lead to larger calibration errors.

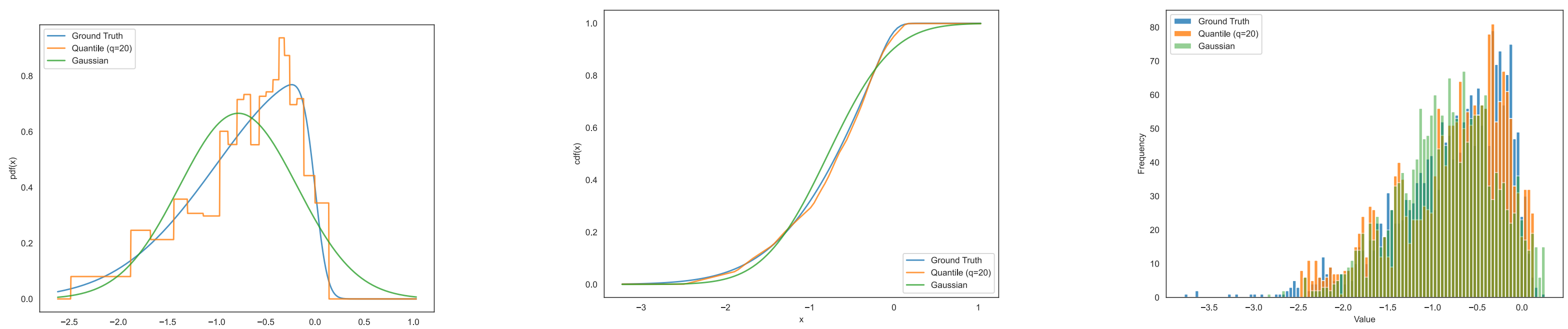
Table 3.1: Statistical metrics of distributions estimated by three methods on synthetic datasets with sample size ranging from 50 to 500. For each method and sample size, the mean, standard deviation, and KL divergence are reported to assess the estimation performance.

Sample Size	**Estimator**	**Mean**	**Standard Deviation**	**KL Divergence**
50	Gaussian	-0.7985	0.6005	0.5727
	Quantile ($\lvert q\rvert = 10$)	-0.7481	0.5503	0.1646
	Quantile ($\lvert q\rvert = 20$)	-0.7440	0.5536	0.2928
100	Gaussian	-0.7989	0.6145	0.6181
	Quantile ($\lvert q\rvert = 10$)	-0.7744	0.5941	0.0953
	Quantile ($\lvert q\rvert = 20$)	-0.7654	0.5798	0.1297
150	Gaussian	-0.7986	0.6100	0.5977
	Quantile ($\lvert q\rvert = 10$)	-0.7860	0.6133	0.0811
	Quantile ($\lvert q\rvert = 20$)	-0.7791	0.5950	0.0948
200	Gaussian	-0.7969	0.6162	0.6227
	Quantile ($\lvert q\rvert = 10$)	-0.7948	0.6347	0.0625
	Quantile ($\lvert q\rvert = 20$)	-0.7833	0.6050	0.0676
250	Gaussian	-0.7921	0.6127	0.6166
	Quantile ($\lvert q\rvert = 10$)	-0.7936	0.6384	0.0526
	Quantile ($\lvert q\rvert = 20$)	-0.7815	0.6084	0.0576
300	Gaussian	-0.7940	0.6140	0.6168
	Quantile ($\lvert q\rvert = 10$)	-0.8002	0.6521	0.0540
	Quantile ($\lvert q\rvert = 20$)	-0.7876	0.6153	0.0482
350	Gaussian	-0.7919	0.6131	0.6176
	Quantile ($\lvert q\rvert = 10$)	-0.8002	0.6570	0.0507
	Quantile ($\lvert q\rvert = 20$)	-0.7866	0.6188	0.0432
400	Gaussian	-0.7919	0.6131	0.6174
	Quantile ($\lvert q\rvert = 10$)	-0.8041	0.6650	0.0491
	Quantile ($\lvert q\rvert = 20$)	-0.7871	0.6215	0.0388
450	Gaussian	-0.7908	0.6114	0.6121
	Quantile ($\lvert q\rvert = 10$)	-0.8054	0.6668	0.0468
	Quantile ($\lvert q\rvert = 20$)	-0.7888	0.6240	0.0357
500	Gaussian	-0.7922	0.6081	0.5956
	Quantile ($\lvert q\rvert = 10$)	-0.8070	0.6657	0.0459
	Quantile ($\lvert q\rvert = 20$)	-0.7912	0.6219	0.0328
-	Ground Truth	-0.7939	0.6080	0.0000



(a) (b) (c)

Figure 3.2: Visualization of the distributions estimated from 10 quantile levels using a synthetic dataset with 150 samples. The figure includes the estimated PDF (a), CDF (b), and the histogram of 2000 samples drawn from the estimated distribution (c).



(a) (b) (c)

Figure 3.3: Visualization of the distributions estimated from 20 quantile levels using a synthetic dataset with 150 samples. The figure includes the estimated PDF (a), CDF (b), and the histogram of 2000 samples drawn from the estimated distribution (c).

3.4. Acquisition Function and Search Strategy

Finally, we describe the acquisition functions and the aquisition optimization strategies used within the BANANAS-CP framework.

3.4.1. Acquisition Functions

We consider four commonly used acquisition functions. Consistent with the notation in the previous sections, $\hat{f}(a)$ is the predicted performance of architecture a and $\hat{F}_a$ represents the CDF of the estimated distribution of $f(a)$. Then, depending on the acquisition function used, the specific acquisition score can be calculated by:

ITS: A sample is drawn from the distribution at random and its value is seen as the acquistion score for the candidate architecture a.

UCB: The acquisition score is given by $\mu + \gamma \cdot \sigma$ for a Gaussian distribution, where γ is the exploration factor. For non-Gaussian distributions, we follow [9] and generalize the function to a quantile function, i.e., $\hat{F}_a^{-1}(\gamma)$. As in the original formulation, higher values of γ promotes exploration. In our experiments, we set $\gamma = 0.75$ due to these concerns: a) the distribution of model performance is believed to be left-skewed; b) estimates of extreme quantiles are generally based on sparse observations and therefore might be less reliable. A value of 0.75 is likely to offer a reasonable trade-off between exploration and accurate estimation.

PI: The probability of improvements corresponds to $1 - \hat{F}_a^{-1}(f_{max})$, with f_{max} being the highest model performance ever observed.

EI: The expected value of improvements can be written as $\mathbb{E}[\max(0, f(a) - f_{max})]$, with f_{max} being the highest model performance ever observed.

3.4.2. Acquisition Optimization Strategy

In parallel to the settings in [33] (see Section 2.1.2), we compare three different approaches for constructing a set with 100 [1] candidates in order to compute the acquisition scores. The motivations and the specific approaches are described below:

Mutation We investigate the mutation-based search strategy because this approach demonstrates the best performance in [33]. In line with their approach, the candidates are selected by randomly changing one operation or one edge of the k best models that have been found so far, where k is a search hyperparameter with the default value of 2.

[1] We have conducted preliminary experiments using 1,000 candidate samples as well. The results indicate that increasing the sample size does not lead to significant improvements in performance. Considering the size of the search space (NAS-Bench-201), and the required computational time, the candidate set size is fixed at 100 for all subsequent primary experiments.

Random Sampling This approach is explored under the assumption that globally sampled architectures may improve the quality of the calibration process. As indicated by the name, the candidate set is created by randomly sampling architectures from the entire search space.

Dynamic This approach aims to resemble the "random + mutation" search strategy in [33]. The search process begins with random sampling until utilizing the first half of the search budget, then switches to a mutation-based strategy that progressively reduces the number of best ever-found models considered for mutation. To be precise, the number of models to be mutated decreases by 2 every 20 epoch. For instance, in a NAS task with 160 epochs, candidates are picked via random sampling for the first 80 epochs. Starting from epochs 80/100/120/140, the candidates are selected by mutating the best 8/6/4/2 models, respectively.

4. Experiments and Results

This chapter describes the performance of the methods presented in Chapter 3 applied to the datasets described in Chapter **??**. We first describe the general setups common to all experiments, then present the configuration tuning strategy together with the implementation details.

4.1. Setups and Implementation

Consistent with [33], each algorithms is assigned with a search budget of 150 epochs. We run 50 trials of each algorithm and average the results.

nuber of candiates. parallel search s

..declare which codes are from the NASlib library. Validation accuracy is a commonly used supervision signal for NAS.

4.2. Baseline

SCP with the ensemble predictor serves as the baseline calibrated strategy.

5. 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.

6. Future Work

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Acronyms

BANANAS	Bayesian Optimization with Neural Architectures for Neural Architecture Search
BANANAS-CP	BANANAS with Conformal Prediction
Bootstrap-CP	Conformal Prediction with Bootstrapping
CDF	Cumulative Distribution Function
CP	Conformal Prediction
CQR	Conformal Quantile Regression
CrossVal-CP	Conformal Prediction with Cross-validation
DAG	Directed Acyclic Graph
EI	Expected Improvements
FCP	Full Conformal Prediction
FNNs	Feedforward Neural Networks
ITS	Independent Thompson Sampling
LOO	leave-one-out
NAS	Neural Architecture Search
PDF	Probability Density Function
PI	Probability of Improvements
RMSCE	Root Mean Squared Calibration Error
SCP	Split Conformal Prediction
TS	Thompson Sampling
UCB	Upper Confident Bound

A. Program Code and Data Resources

The source code and a documentation are available at the GitHub repository: https://github.com/chengc823/Thesis. The datasets used for experiments and algorithm evaluations are sourced from the NASLib repository.

In case of access or permission issues to the private repository, please reach out at: chechen@mail.uni-mannheim.de.

B. 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	+
ChatGPT	Debugging LaTeX syntax errors	Equation	+
ChatGPT	Rendering LaTeX tables from Python frame	Tables	+

Unterschrift
Mannheim, den 31.07.2025