Inductive Bias in Model Selection

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Abstract

This paper is devoted to the problem of choosing the architecture of suboptimal models in multitask learning paradigm. The assumption is introduced that when searching for models in the search space of a sufficiently high dimension, the resulting model architecture will reflect the features of the analyzed data, which can be interpreted as an inductive bias of the model. An automatic procedure can be employed using evolutionary method of searching for a model based on symbolic regression algorithms. Model trains independently on a set of given datasets of a particular class.

Keywords model selection · evolutionary algorithm

1 Introduction

The concept of inductive bias is a fundamental tenet in the realm of machine learning, encapsulating the core assumptions that underpin the methodology adopted by a particular model in its predictive endeavours, extending beyond the boundaries of explicitly observed data. Understanding and leveraging inductive bias is essential for enhancing model performence, especially in complex environments where data may exhibit diverse characteristics.

In recent years, the field of machine learning has experienced rapid advancements driven by the development of sophisticated algorithms and architectures capable of tackling a wide range of tasks, from natural language processing to computer vision. However, the design and optimization of these models often require significant expertise and resources, leading to the rise of automated machine learning (AutoML) systems. These systems aim to alleviate the burden of manual model selection and tuning, enabling broader accessibility to machine learning techniques.

One notable approach is AutoML-Zero, which autonomously constructs models using a genetic programming framework, assembling them from fundamental mathematical operations [1]. This method represents a significant departure from traditional model selection paradigms, which typically rely on predefined structures or human intuition. By allowing the model architecture to emerge organically from the data, AutoML-Zero minimizes biases introduced by prior knowledge, potentially leading to the discovery of novel architectures better suited to the task at hand.

The concept of inductive bias plays a crucial role in model generalization. Different datasets often possess unique distinguishing features that can be exploited for improved performance. For instance, models trained on image data may benefit from biases related to spatial hierarchies, while those handling sequential data, such as time series or text, may rely on temporal dependencies. Recognizing and systematically integrating these biases into the model selection process can facilitate the identification of suboptimal yet effective architectures.

In this paper, we investigate how inductive biases inherent in the data can inform model selection within the multitask learning framework. We propose an automated approach that leverages evolutionary algorithms in conjunction with symbolic regression to explore a diverse range of model architectures. By allowing models to train independently on various datasets within a specific class, our methodology aims to enhance generalizability and adaptability while reducing the need for extensive manual tuning.

The experiments are focused on a range of datasets that capture different characteristics, enabling a robust evaluation of how well our models generalize across tasks. The goal is to provide insights into the relationship between inductive bias and model architecture.

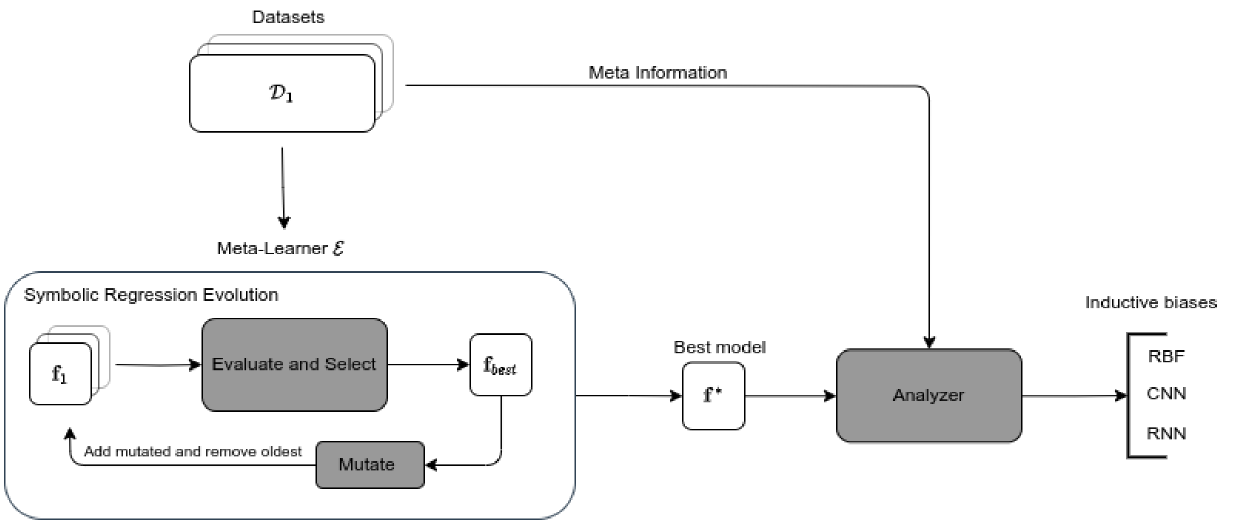

Figure 1: Pipeline.

2 Problem statement

Let $\mathfrak{T} = \{T_1, T_2, \ldots, T_n\}$ be a set tasks. Each task T_i has its corresponding dataset $\mathfrak{D}_i$, where $\mathfrak{D}_i = \{(\mathbf{x}_j, y_j)\}_{j=1}^{N_i}$ represents N_i examples of input-output pairs. We will denote a meta-learner as $\mathcal{E}$ and an analyzer as $\mathbf{f}_{\text{CLF}}$. The meta-learner $\mathcal{E}$ constructs a candidate models given the datasets. Inductive bias then infered by the $\mathbf{f}_{\text{CLF}}$.

2.1 Meta-Learner

Let $\mathfrak{F}$ be the family of all models. The model is defined by three functions: `Setup`, `Learn` and `Predict`. The meta-learner $\mathcal{E} : 2^{\mathfrak{D}} \to \mathfrak{F}$ is based on AutoML-Zero algorithm. The algorithm incorporates evolutionary search method on training datasets to generate candidate models, which are then selected and mutated based on their accuracy on test datasets. Evolutionary search is conducted as follows:

- Initialization: Generate an initial population of models $\mathcal{F}_0 \subset \mathfrak{F}$ of size P.
- Evaluation: During each evolution cycle asses each model $f \in \mathcal{F}_t$ using accuracy metric, where $\mathcal{F}_t$ is the population at t-th cycle.
- Mutation: Select the best model and mutate it to product a child model. To keep the population size fixed, the oldest model is replaced by the child model. (details about mutation can be put in apendix)
- Termination: Repeat for C cycles and select the best model f^* accross all cycles.

The best model is found based on mean accuracy. If we have m_2 test datasets then the metric on a set of tasks can be computed as

$$\text{mACC}(f, \mathfrak{D}) = \frac{1}{m_2} \sum_{i=1}^{m_2} \text{ACC}(f, \mathfrak{D}_i) = \frac{1}{m_2} \sum_{i=1}^{m_2} \sum_{j=1}^{N_i} \frac{[f(\mathbf{x}_j) = y_j]}{N_i}$$

Hence, the optimization in this stage can be written as

$$f^* = \arg\max_{f \in \mathfrak{F}} \text{mACC}(f, \mathfrak{D}).$$

2.2 Analyzer

Given the best model $\mathbf{f}^*$ we can infer an inductive bias of the tasks. We categorized inductive biases into three categories: RBF, CNN and RNN. The inference is done by analyzer $\mathbf{f}_{\text{CLF}}$ which was selected to be [MODEL] model.

By getting an internal represention of the best model f^*, i.e. the funcitons comprising `Setup`, `Predict` and `Learn`, we use [MODEL] to infer the inductive bias hidden in the representation.

OR. Try to make map internal representation of the funcitons into latent space. Maybe functinos with the same inductive biases will cluster?

3 Model description

4 Computational experiment

4.1 Data

Suppose $\{\mathfrak{D}_1, \mathfrak{D}_2, \ldots, \mathfrak{D}_n\}$ are the datasets. The datasets have same inductive bias but they differ from each other by some property. We select m_1 elements from each dataset to form a set of training datsets $\mathfrak{D}_{train}$, and from a remaining part we get a set of testing datasets $\mathfrak{D}_{test}$.

4.2 Experiments

We conducted experiment for binary classification task using concentrated circles datasets. The datasets have different center position of the circles and noise parameters.

4.3 Results of the experiments

5 Conclusion

References

[1] Esteban Real, Chen Liang, David So, and Quoc Le. Automl-zero: Evolving machine learning algorithms from scratch. In *International conference on machine learning*, pages 8007–8019. PMLR, 2020.