Efficient Automated Deep Learning for Time Series Forecasting

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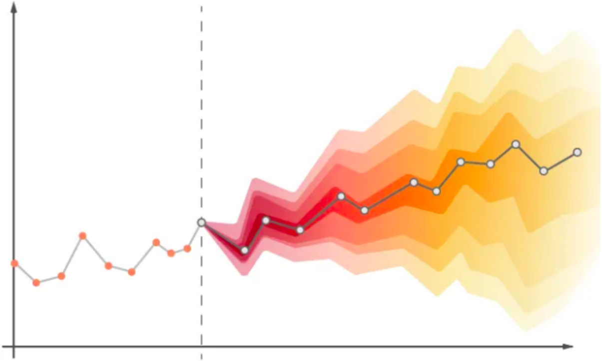
Contents

1. The TSF Problem

Time series forecasting (TSF) is the task of predicting future values of a given sequence based on previously observed values.



The TSF problem may be essentially identified by the following aspects:

- **Prediction objective**: point forecasting vs probabilistic forecasting
- **Forecast horizon**: short-term vs long-term forecasting
- **Input-Output dimension**: univariate vs multivariate forecasting
- **Forecasting task**: single-step vs multi-step forecasting

Nowadays, the TSF problem is usually faced with **Deep Learning models** (RNN, LSTM). However, the design of these models is a challenging task due to:

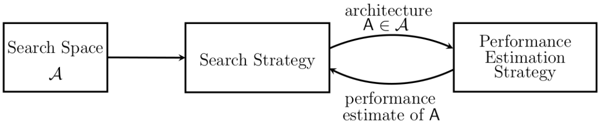
- **model architecture**: the choice of the model architecture is crucial for the performance of the model
- **hyperparameters**: the selection of the optimal hyperparameters is also extremely relevant for the model's performance
- **computational cost**: the search for the best model architecture and hyperparameters is resource expensive

To deal with these issues, the authors proposed a new framework for **Automated Deep Learning for TSF**.

2. NAS & HPO

Neural Architecture Search (NAS) is a technique that automates the design of neural network architectures and it is based on three main components:

- **Search Space** defines which architectures can be considered
- **Search Strategy** details how to explore the search space, dealing with the exploration-exploitation trade-off
- **Performance Estimation Strategy** is the process to estimate the architecture performance on test data



Hyperparameter Optimization (HPO) is the process of finding the best set of hyperparameters for a given model.

Bayesian Optimization (BO) is a **sample efficient method** for HPO that is based on two main components:

- a **probabilistic surrogate model** to approximate the objective function (usually a Gaussian Process or a Tree-based model)
- an **acquisition function** to deal with the trade-off between exploration and exploitation (e.g., Expected Improvement, Confidence Bounds, etc.)

The **Combined Algorithm Selection and Hyperparameter** (CASH) approach consists of a sequential learning process that first selects the most promising algorithms and then optimizes for their optimal hyperparameter configurations.

In the context of DL models, a CASH approach:

- uses NAS to search over a variety of architectures (the search process is usually performed via BO with Random Forest as surrogate model, since the search space is conditional and high-dimensional)
- adopts BO to optimize the hyperparameters of the models

3. AutoDL for TSF

Recent years have witnessed great efficiency improvements in AutoDL systems but little attention has been paid to general automatic framework for TSF.

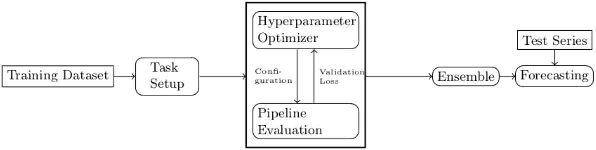
The authors proposed a new framework for **Automated Deep Learning for TSF** that:

- uses **NAS** to search over a variety of state-of-the-art TSF architectures
- adopts **BO** to optimize the hyperparameters of the models (with a **CASH** approach)
- explores **multi-fidelity optimization** to reduce the computational cost of the search process

Automatic Forecasting Pipeline

The proposed framework is based on a **forecasting pipeline** that:

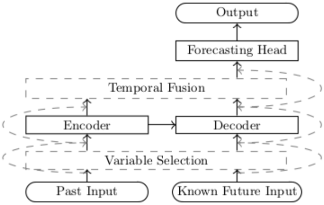
- first, it automatically **prepares the data** and splits each sequence into training, validation, and test sets
- then, the optimizer **searches for desirable architectures and hyperparameters** from the search space
- finally, a **weighted ensemble** of the top k selected configurations is used to evaluate the final predictions on the test set



Search Space

SOTA architectures for TSF can be decomposed into two parts:

- the **encoder** processes the input sequence (past target values) and embeds them into a latent space
- the **decoder** processes the latent embedding and future features and generates a sequence of scalar values through the output layer



Search Space

Based on encoder-decoder architectures, the final search space contains many TSF algorithms, such as NBEATS, DeepAR, TFT.

Encoder		Decoder	auto-regressive	Architecture Class
Flat Encoder	MLP	MLP	No	Feed Forward Network
	N-BEATS	N-BEATS	No	N-BEATS [46]
Seq. Encoder	RNN/Transformer	RNN/Transformer	Yes	Seq2Seq [9]
			No	TFT [38]
		MLP	Yes	DeepAR [50]
			No	MQ-RNN [57]
	TCN	MLP	Yes	DeepAR [50]/WaveNet [45]
			No	MQ-CNN [57]

Network encoder may be sequential or flat.

Forecasting architecture may be autoregressive or not.

Hyperparameter Optimization

The loss function is optimized on the validation set via **BO**.
Since training deep neural networks requires lots of computational resources, **multi-fidelity optimization** is used to reduce the computational cost of the search process:

- it allows to train the model with different **budget types** (number of epochs, time series length and number of series)
- starting with the lowest budget setup and gradually assigning higher budgets to well-performing configurations
- it prevents the optimizer from investing too many resources on the poorly performing configurations and allows to **focus on the most promising** ones
- it may introduce **bias** in the performance estimation

4. Conclusions

- The authors proposed a framework for AutoDL in the context of TSF to efficiently search for the best model architectures and hyperparameters
- The search space is based on state-of-the-art TSF algorithms formulated as an encoder-decoder architecture
- Empirical results show that the proposed framework is able to outperform the state-of-the-art methods on a variety of datasets
- The optimal choice of budget type is dataset specific and the most important hyperparameters are related to the optimizer of the neural network and its learning rate

Bibliografy

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Thank you!