Efficient Automated Deep Learning for Time Series Forecasting

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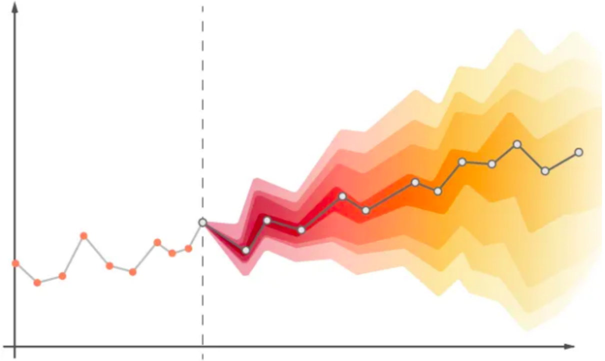
Contents

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

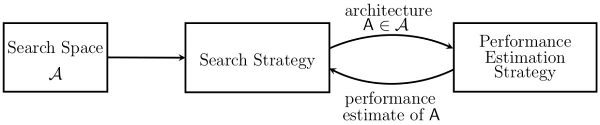
For this reason, the authors proposed a new open source framework for **Automated Deep Learning for TSF** that:

- 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.

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

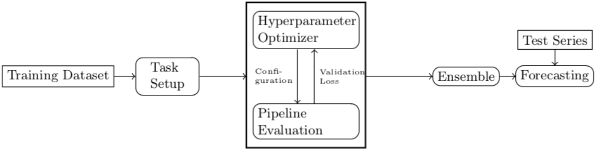
3. AutoDL for TSF

The application of NAS to the TSF problem is a relatively new research field.

The Forecasting Pipeline

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

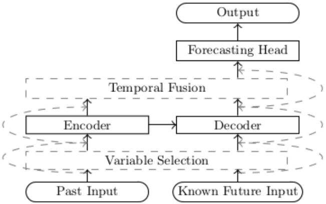
- first, it automatically **prepares the data** and splits each sequence into training, validation, and test sets
- then, the optimizer **searches for desirable architectures and hyperparameters** from the search space
- finally, a **weighted ensemble** of the top k selected configurations is used to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



The Search Space

SOTA architectures for TSF can be decomposed into three 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.
The **forecasting head** is the output layer and takes the decoder's output to generate a sequence of scalar values.



The 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 hyperparameters of the models are optimized via a **CASH approach**.

The loss function (usually MAE or MASE) is optimized on the validation set via **BO**, using **Random Forest** as surrogate model.

Multi-fidelity optimization is used to reduce the computational cost of the

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 the most recent SOTA TSF algorithms formulated as an encoder-decoder architecture
- Empirical results show that the proposed framework is able to outperform the SOTA 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!