

A Unified Hyperparameter Optimization Pipeline for Transformer-Based Time Series Forecasting Models

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Abstract—Transformer-based models for time series forecasting (TSF) have attracted significant attention in recent years due to their effectiveness and versatility. However, these models often require extensive hyperparameter optimization (HPO) to achieve the best possible performance, and a unified pipeline for HPO in transformer-based TSF remains lacking. In this paper, we present one such pipeline and conduct extensive experiments on several state-of-the-art (SOTA) transformer-based TSF models. These experiments are conducted on standard benchmark datasets to evaluate and compare the performance of different models, generating practical insights and examples. Our pipeline is generalizable beyond transformer-based architectures and can be applied to other SOTA models, such as Mamba and TimeMixer, as demonstrated in our experiments. The goal of this work is to provide valuable guidance to both industry practitioners and academic researchers in efficiently identifying optimal hyperparameters suited to their specific domain applications. The code and complete experimental results are available on GitHub¹.

Index Terms—Transformer, Time Series, Forecasting, Benchmark, Hyperparameter Optimization (HPO), Deep Learning, Unified Pipeline

I. INTRODUCTION

Time series forecasting (TSF) is important for decision making across diverse practical domains, making it a continuously evolving field. Over time, TSF models have progressed from classic approaches, such as auto-regressive-moving-average (ARMA) models and exponential smoothing, to more sophisticated deep learning models, largely due to rapid advancements in computational capabilities [6, 17]. Among these advancements, deep learning models, particularly transformer models, have demonstrated significant potential in improving the accuracy and efficiency of TSF. However, these models often depend on a wide range of hyperparameters, and optimizing

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¹https://github.com/jingjing-unilu/HPO_transformer_time_series

them typically requires substantial expertise. Thereby, these models increase the technical barriers for users attempting to apply these models to different datasets with varied hyperparameter configurations [8, 33, 15]. As a result, hyperparameter optimization (HPO) become increasingly critical for ensuring the effective use of transformer models in TSF.

In the context of machine learning and deep learning, HPO refers to the process of selecting an optimal set of hyperparameters for a model to minimize a predefined loss function with given specific dataset [5]. While several studies have explored HPO for various machine learning models and TSF applications, research specifically focused on HPO for transformer-based TSF models remains limited. To address this gap, we introduce a unified HPO pipeline designed specifically for transformer-based TSF models. Additionally, we evaluate several state-of-the-art (SOTA) models on standard datasets to provide practical insights and examples of the pipeline's effectiveness.

The structure of the paper is as follows: Sec. II reviews the background and related work; Sec. III details the experimental setup; Sec. IV presents the results and analysis; and Sec. V concludes the paper with future directions. Our aim is to enhance the reproducibility, fairness, and performance of TSF models across diverse datasets and domains. The key contributions of this work are as follows:

- 1) We introduce a Hyper-Parameter Tuning pipeline specifically designed for transformer-based and other TSF models.
- 2) We benchmark standard datasets using various SOTA TSF models, including transformer-based models, Mamba [9], and TimeMixer [23].
- 3) We perform a comprehensive analysis of the experimental results.

II. BACKGROUND AND RELATED WORK

A. Transformer-based Time Series Forecasting

The Transformer model has emerged as a good option for time series forecasting (TSF) due to its excellent ability to capture long-range dependencies. Several transformer-based forecasting models have been developed to address various forecasting challenges. Informer [35] and Autoformer [28] pioneers the adaptation of transformer components for time series applications. Subsequently, the Crossformer model [34] focuses on capturing cross-time and cross-dimensional dependencies to enhance multivariate time series forecasting. Meanwhile, the Non-stationary Transformer [14] addresses issues related to stationarity in forecasting tasks. Following this, PatchTST [16] employs patching and channel-independent architectures to effectively capture both local and longer lookback information. The iTransformer [13] reconfigures the traditional transformer structure, offering an alternative approach for time series forecasting. Comprehensive surveys [2, 25, 30] provide an overview of transformer models tailored for TSF. Additionally, researchers have begun to apply transformer-based TSF methods in finance [27, 26]. Furthermore, emerging techniques and models for time series forecasting include graph representation learning [11], Large Language Models (LLMs) [12], Mamba [9], and TimeMixer [23].

B. HPO for Transformer

Hyperparameter optimization (HPO) search algorithms include Grid Search, Random Search, Bayesian Optimization (BO), Tree Parzen Estimators (TPE), and others [33, 22]. HPO is a critical component of machine learning, as it enables models to select the optimal set of hyperparameters to maximize performance on a given dataset. Some researchers have addressed HPO in the context of common machine learning models [5, 32], and discussions surrounding HPO for deep learning and neural networks have also emerged. Generally, hyperparameters in deep learning can be classified into two categories: those related to model architecture and those associated with training and optimization. In works related to model architecture, a recent survey [3] explores neural architecture search (NAS) benchmarks, highlighting the need for efficient search algorithms. Additionally, another survey [4] summarizes the NAS landscape for Transformers and their associated architectures, specifically discussing HPO in autotransformer [19] for time series classification tasks. However, the exploration of HPO for Transformers in time series forecasting tasks remains insufficient.

C. HPO for Time Series Forecasting

HPO is crucial for improving forecast performance and mitigating overfitting issues in time series forecasting. A review [15] identifies hyperparameter optimization (HPO) as one of the five key components of the time series forecasting pipeline, concluding that the grid search method is the most widely used in automated forecasting frameworks. Additionally, evolutionary optimization and Bayesian Optimization are often employed in high-complexity training processes. The

paper [7] presents hyperparameter tuning algorithms specifically for Long Short-Term Memory (LSTM) networks, aiming to efficiently determine the optimal set of hyperparameters. Furthermore, another paper [20] proposes a distributed HPO approach for time series forecasting based on electricity dataset. Researchers [10] investigate the three hyperparameter tuning toolkits Scikit-opt, Optuna and Hyperopt, and then apply these toolkits to Convolutional Neural Networks (CNN) and LSTM models for wind power prediction. Recently, the paper [21] introduced an automatic hyperparameter tuning framework for the Temporal Fusion Transformer (AutoTFT) model (for multi-horizon time series forecasting). Despite these advancements, research focused on HPO for various transformer-based time series forecasting models across different model on datasets remains limited.

III. EXPERIMENTS

In this study, we perform hyperparameter optimization for long-term time series forecasting. The primary objective is to identify a set of hyperparameter values that minimizes forecasting errors across different models.

A. Dataset and Metrics

We utilize widely-used open-source datasets for long-term time series forecasting, including ETTh1, Weather and Electricity. The evaluation metrics employed in this experiment are Mean Squared Error (MSE) and Mean Absolute Error (MAE), which are commonly used to assess model performance, as noted in the survey [30]. A summary of the datasets is provided in Tab. I, and detailed descriptions of the datasets can be found in related works [28, 35].

TABLE I: Summary of three datasets.

Datasets	ETTh1	Weather	Electricity (ECL)
Variables	7	21	321
Timesteps	17420	52696	26304

B. Environment and Configuration

All experiments in this study were conducted on a single Nvidia TU02 GPU.

1) *Model and its Setting:* For our case study, we randomly selected four transformer-based TSF models: Autoformer [28], Crossformer [34], Non-Stationary Transformer [14], and PatchTST [16]. Additionally, we include other state-of-the-art (SOTA) models, such as Mamba [9] and TimeMixer [23], for comparison. For model settings, we selected the long-term forecasting task as the primary focus of this paper. Additionally, while we arbitrarily chose a prediction length of 96 as a use case, other prediction lengths (192, 336, 720) can be implemented in a similar fashion. In addition, the evaluation metrics used are Mean Squared Error (MSE) and Mean Absolute Error (MAE), which are standard measures for model performance.

TABLE II: Parameters for Different Models. NOTE: 1)DF:Default

Parameter	Module	Default	PatchTST				Crossformer				Autoformer				Non-stationary_Transformer				Lowest	Highest
			ETTh1	weather	electricity	traffic	ETTh1	weather	electricity	traffic	ETTh1	weather	electricity	traffic	ETTh1	weather	electricity	traffic		
data	# data loader	ETTh1	custom	custom	custom	custom	ETTh1	custom	custom	custom	ETTh1	custom	custom	custom	ETTh1	custom	custom	custom	-	-
features	# data loader	'M'	M	M	M	M	M	M	M	M	M	M	M	S	M	-	-	96	96	
seq_len	# forecasting task	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96
label_len	# forecasting task	48	48	48	48	48	48	48	48	48	48	48	48	48	48	48	48	48	48	48
pred_len	# forecasting task	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96	96
e_layers	# model define	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	2
d_layers	# model define	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
factor	# model define	1	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	1	3
enc_in	# model define	7	7	21	321	862	7	21	321	862	7	21	321	862	7	21	321	862	7	862
dec_in	# model define	7	7	21	321	862	7	21	321	862	7	21	321	862	7	21	321	862	7	862
c_out	# model define	7	7	21	321	862	7	21	321	862	7	21	321	862	7	21	321	862	7	862
d_model	# model define	512	DF	DF	DF	512	DF	DF	DF	512	DF	DF	DF	DF	DF	DF	DF	DF	32	2048
d_ff	# model define	2048	DF	DF	DF	512	DF	DF	DF	512	DF	DF	DF	DF	DF	DF	DF	DF	32	2048
top_k	# model define	5	DF	DF	DF	5	DF	DF	DF	5	DF	DF	DF	DF	DF	DF	DF	DF	5	5
n_heads	# model define	8	2	4	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	2	8
des	# model define	0.1	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	0.1	0.1
des	# optimization	'test'	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	Exp	-	-
train_epochs	# optimization	1	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	1	1
batch_size	# optimization	10	DF	3	DF	DF	DF	1	DF	DF	DF	2	DF	3	DF	3	DF	3	1	10
learning_rate	# optimization	0.0001	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	4	128
p_hidden_dims	# de-stationary projector params	[128,128]	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	0.0001	0.0001
p_hidden_layers	# de-stationary projector params	2	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	DF	2	256

2) *HPO Setting*: During the hyperparameter tuning process, the model with the lowest validation loss (MSE) is defined as the best-performing model. Each model undergo 20 trials on each dataset to tune hyperparameters. We utilize OptunaSearch (a variant of Tree-structured Parzen Estimator, TPE) as an example of search algorithms. Our pipeline also supports commonly used search algorithms such as random search, grid search, and Bayesian optimization. As a hyperparameter tuning tool, we utilized Ray Tune², a scalable tool designed to optimize model performance efficiently. Additionally, Weights & Biases³ is applied to visualize the hyperparameter tuning processes and outcomes. The code of this paper is built upon the Time Series Library [29].

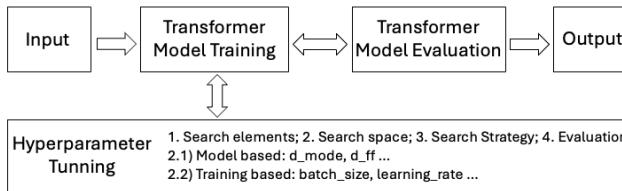


Fig. 1: HPO pipeline for Transformer-based forecasting

C. HPO Pipeline

The hyperparameter optimization (HPO) pipeline is depicted in Fig. 1. The process begins with feeding data into the model, followed by the simultaneous execution of model training and hyperparameter tuning. Once the training is completed, the model is evaluated, and the results are output. In line with the Neural Architecture Search (NAS) framework, four key components are integral to the hyperparameter tuning process: collecting primitive search elements (hyperparameters), designing the search space, selecting the search algorithm, and evaluating performance to determine the optimal model or network [4]. OptunaSearch is employed in the experiments as the search algorithm, and the evaluation of results is discussed in Sec. IV. Therefore, we emphasize the collection of primitive hyperparameters and the design of the search space in this section.

²<https://github.com/ray-project/ray>

³<https://github.com/wandb/wandb>

TABLE III: Common Parameters in this Experiments

Parameter	Module	Default	Lowest Value	Highest Value	Searching Space
d_ff	model define	2048	32	2048	[16,32,64,128,256,512,1024,2048,4096]
d_layers	model define	1	1	1	[1,2]
d_model	model define	512	32	2048	[16,32,64,128,256,512,1024,2048,4096]
e_layers	model define	2	1	2	[1,2,3]
factor	model define	1	1	3	[1,2,3,4]
n_heads	model define	8	2	8	[2,4,8,16]
batch_size	optimization	32	4	128	[4, 16, 32, 64, 128, 256]
learning_rate	optimization	0.0001	-	-	[0.00001, 0.0001, 0.001]
train_epochs	optimization	10	1	10	[1,2,3,4,5,6,7,8,9,10,11]

1) *Hyperparameters and Search Spaces*: We first gather all hyperparameters from the Time Series Library⁴, and then review the parameters used across different models as shown in Tab. II (Mamba and TimeMixer follow the same lowest and highest value). Most of the parameters are assigned default values. For the hyperparameter tuning experiments, we select common parameters shared by the models. The selected parameters and corresponding search spaces are presented in Tab. III. These hyperparameters are divided into two categories: “model define” and “optimization (training)” groups. The ‘optimization (training)’ group includes parameters that influence the speed of convergence, while the “model define” group comprises hyperparameters that determine the learning capacity of the model. The parameters in the “model define” group are illustrated in Fig. 2. To define the search space, we first identified the minimum and maximum values for each parameter across models. The search space range is then extended by setting the lower bound one step below the minimum value and the upper bound one step above the maximum value.

IV. RESULTS AND ANALYSIS

In our experiments, each model is subjected to 20 trials per dataset, employing the OptunaSearch algorithm for hyperparameter optimization. A total of 357 trials are conducted (6 models * 20 trials * 3 datasets, minus 3 unexecuted cases). We analyze these experiments by examining the best performance of each model and investigating the behavior of hyperparameters.

A. Best results on different datasets

Tab. IV presents the best results for each model across the datasets. **bold** numbers indicate the best performance,

⁴<https://github.com/thuml/Time-Series-Library>

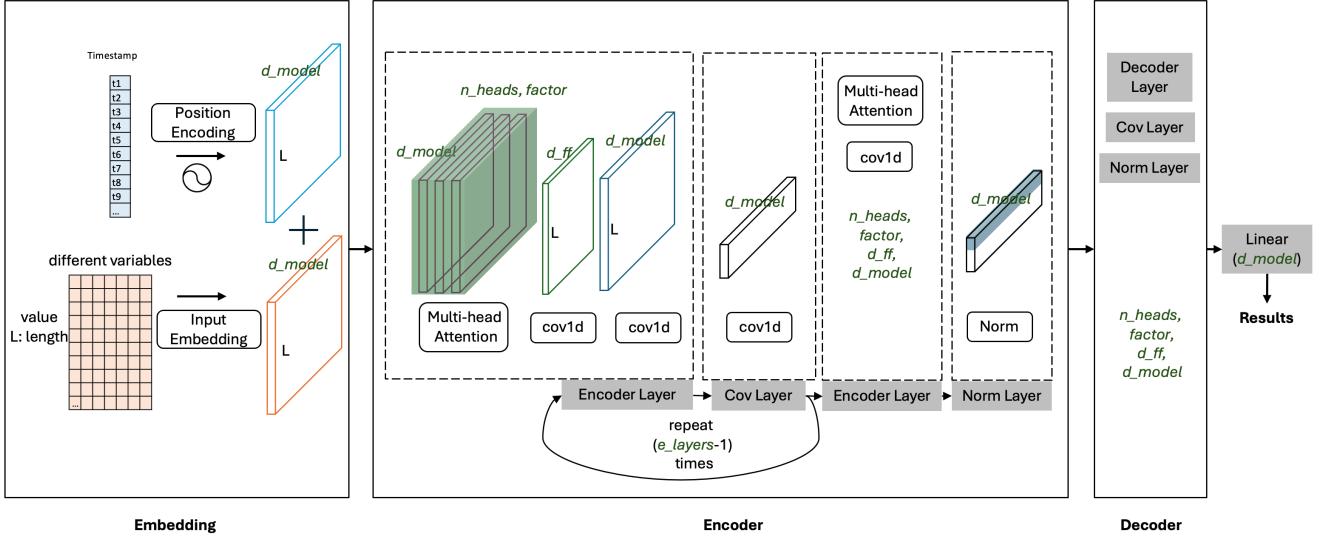


Fig. 2: Common Parameters in the Transformer

while underline numbers denote the second-best performance. For the ETTh1 dataset, TimeMixer achieved the best results. In contrast, for the Weather and ECL datasets, Crossformer demonstrates better performance even it is a time-consuming model. The learning curve in Fig. 3 illustrates the performance behavior of each model. The details are as follows.

TABLE IV: Best result of different models on different datasets

Model	ETTh1			Weather			Electricity (ECL)		
	MSE	MAE	Time	MSE	MAE	Time	MSE	MAE	Time
PatchTST	0.3852	0.3974	654	0.1735	0.2158	621	0.1739	0.2699	532
Crossformer	0.4149	0.4412	62	0.1527	0.2278	3458	0.1347	0.2319	8647
Autoformer	0.4466	0.4559	136	0.2857	0.3552	190	0.1981	0.3121	3330
Nons. Trans.	0.5515	0.5126	106	0.1867	0.2342	225	0.1683	0.2729	284
Mamba	0.4701	0.4416	499	0.1942	0.2413	481	0.1691	0.2719	2643
TimeMixer	0.3815	0.3967	128	0.1614	0.2088	4626	0.1747	0.2648	2994

1) *ETTh1 dataset*: Fig. 3a shows that in all models, including the best-performing TimeMixer, the validation loss exceeds the training loss, suggesting underfitting. This indicates that the models have not sufficiently captured the underlying patterns in the training data. From a hyperparameter tuning perspective, increasing the number of epochs or the model's complexity could improve performance. From a data perspective, noise reduction and feature engineering may also help [31, 1, 30, 24].

2) *Weather dataset*: Crossformer achieved the best performance on the Weather dataset, but it was trained for only one epoch, suggesting the need for further hyperparameter tuning. Fig. 3b indicates that most models are underfitting and require additional tuning. However, Autoformer showed slight overfitting, as its validation loss began to increase after initially decreasing. Overfitting suggests that the model cannot generalize well to new data, so reducing model complexity, employing early stopping, or using dropout techniques would be beneficial in future hyperparameter tuning efforts.

3) *ECL dataset*: On the ECL dataset, Crossformer again demonstrated the best performance (see Table IV). As shown in Fig. 3c, the model performed well, with a small difference

between training and validation loss after both decreased. While the results are promising, further hyperparameter tuning can still be conducted to improve the model capability and performance.

B. Hyperparameter and Model Metric

To understand the relationship between hyperparameters and model performance, we map hyperparameter values to validation loss using parallel coordinate plots (lower validation loss means better performance). This approach help us identify the best and worst hyperparameter ranges for each model in further tuning. However, we notice that some models crash due to out-of-memory (OOM) errors, as shown in Tab. V, particularly with the ECL dataset (which has 321 variables). The high number of variables make models such as Crossformer, PatchTST, and TimeMixer sensitive to hyperparameters, resulting in OOM errors. Mamba also encountered a high failure rate, with nearly 50% of trials crashing. To mitigate these OOM errors in the future, we analyze the OOM case in ECL firstly and then continue the analysis of ETTh1 and Weather dataset. All trials' results and parallel coordinate plots are available via GitHub.

TABLE V: Out-of-Memory Rate

Models	ETTh1	Weather	ECL
Autoformer	10%	10%	10%
Crossformer	5%	25%	35%
Nons._Trans.	10%	0%	10%
PatchTST	0%	0%	40%
Mamba	50%	53%	40%
TimeMixer	10%	40%	85%

1) *Dataset: Electricity (ECL)*: During hyperparameter tuning, all models experience crash cases on the ECL dataset. Tab. VI summarizes the models that crashed under the training and model-related parameters ($batch_size$, d_model , d_ff). For instance, the Autoformer model encountered OOM errors when the $batch_size$ is set to 256 while

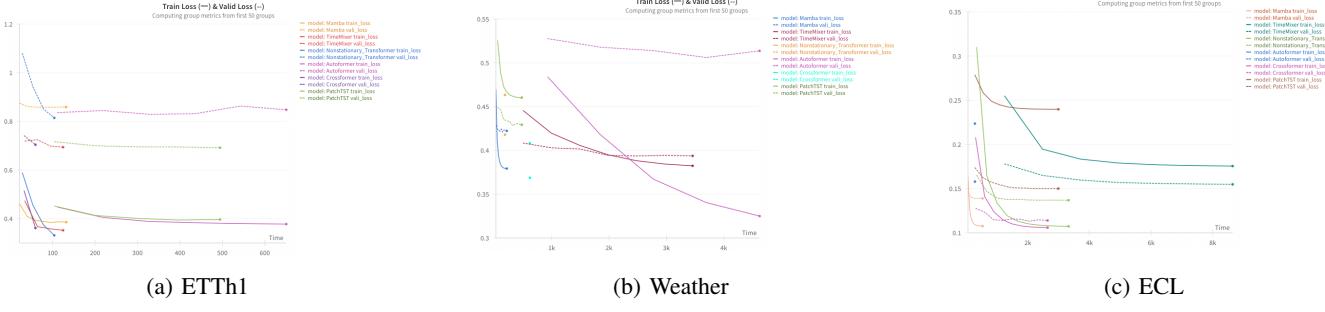


Fig. 3: Training loss and validation loss on each model’s best performance case in experiments

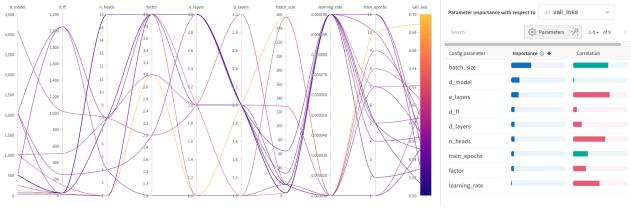


Fig. 4: Parallel coordinates plot on Weather dataset: Autoformer without outlier

$\max(d_model, d_ff) \geq 2048$ and $\min(d_model, d_ff) \geq 16$ (both d_model and d_ff influence the model size). Therefore, hyperparameter tuning process requires more GPU memory or smaller batch sizes [18] for the dataset like ECL.

TABLE VI: Out-of-Memory Case (ECL)

Model	Batch Size	Max(d_model, d_ff)	Min(d_model, d_ff)
Autoformer	256	$>=2048$	$>=16$
Crossformer	128	$>=2048$	$>=256$
Crossformer	256	$>=2048$	$>=32$
Nons. Trans.	128	$>=4096$	$>=16$
PatchTST	32	$>=4096$	$>=1024$
PatchTST	64	$>=4096$	$>=512$
PatchTST	128	$>=2048$	$>=64$
PatchTST	256	$>=1024$	$>=32$
Mamba	4	$>=2048$	$>=64$
Mamba	16	$>=2048$	$>=32$
Mamba	32	$>=4096$	$>=32$
Mamba	64	$>=1024$	$>=32$
Mamba	256	$>=4096$	$>=16$
TimeMixer	16	$>=512$	$>=128$
TimeMixer	32	$>=256$	$>=32$
TimeMixer	64	$>=128$	$>=64$
TimeMixer	128	$>=256$	$>=32$
TimeMixer	256	$>=512$	$>=128$

2) *Dataset: ETTh1:* ETTh1, the smallest dataset in the experiment, experienced fewer OOM errors during hyperparameter tuning. Fig.5a shows that for Autoformer, $batch_size$, $train_epoch$, and n_head are the most influential hyperparameters. Specifically, lower $batch_size$ (≤ 32), higher $train_epoch$ (≥ 9), and $n_head = 4$ lead to better performance. For Crossformer (Fig.5b), d_model , $learning_rate$, and $factor$ are the top three hyperparameters, with smaller d_model (≤ 512), higher $learning_rate$ (0.001), and higher $factor$ (≥ 3) resulting in better performance. In the Non-Stationary Transformer model (Fig. 5c), $d_model = 32$ and $d_ff \leq 512$ while $n_head = 8$ and $d_layer = 2$ lead to

higher validation loss (bad performance). PatchTST demonstrates that a smaller $learning_rate$ (≤ 0.0001) with a higher $train_epoch$ (≥ 5) reduce validation loss. Mamba, being very sensitive to model size, performs better when $d_ff \leq 128$, reducing both OOM errors and validation loss. TimeMixer achieves better results with a larger $learning_rate = 0.001$. Tab. VII summarizes the top three key parameters for each model. From the table, it is evident that d_model frequently has a significant impact on the performance of transformer-based models. In addition, different transformer-based models exhibit varying sensitivities to training-related parameters. In addition, models like Mamba and TimeMixer are predominantly influenced by training-related parameters such as the number of training epochs and learning rate.

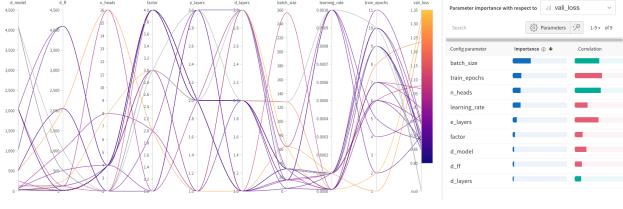
TABLE VII: Top 3 important Parameters in each model (with respect to validation loss in ETTh1 dataset. The number means the importance rank, for example, d_model is the most influential parameter in the Crossformer model.)

model	Model Related				Training Related		
	d_model	d_ff	n_head	$factor$	$batch_size$	$train_epoch$	$learning_rate$
Autoformer	1	3	3	3	1	2	2
Crossformer	2	3	1	3	3	1	1
Non-s. Trans.	2	3	1	3	3	1	1
PatchTST	2	3	1	3	3	1	1
Mamba	1	3	2	2	3	2	1
TimeMixer	1	2	3	2	3	1	1

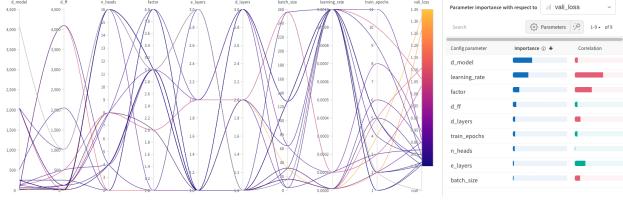
3) *Dataset: Weather:* The weather dataset has more variables and longer sequences compared to ETTh1, making models more prone to OOM errors, particularly in Autoformer and Mamba. To investigate further, we remove outliers from Autoformer’s results and observed that batch size is the most influential parameter (see Fig.4). This finding suggests that larger datasets require smaller batch sizes, which should be a focus in future hyperparameter tuning. For other models, the ranking of parameter importance from the parallel coordinate plots should guide further adjustments. For example, Crossformer’s plot (Fig.6b) suggests that keeping n_head at a higher level (> 8) during future training would improve performance.

V. CONCLUSION

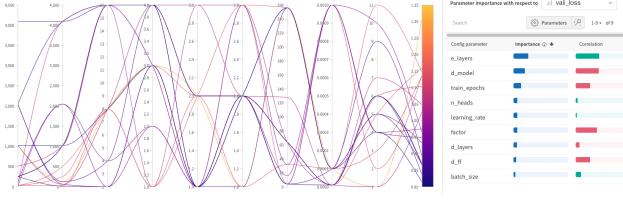
This paper introduces a unified hyperparameter optimization (HPO) pipeline designed for transformer-based time series forecasting (TSF) models. We benchmark several SOTA models, including Autoformer, Crossformer, Non-Stationary Transformer, PatchTST, Mamba, and TimeMixer, across multiple datasets.



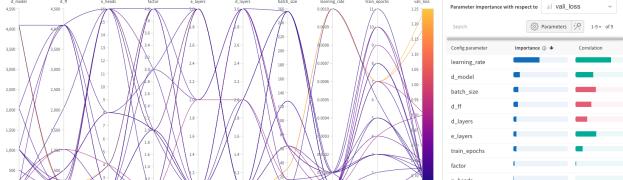
(a) Autoformer



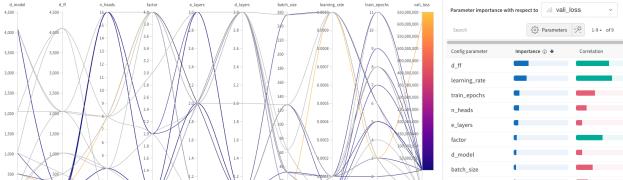
(b) Crossformer



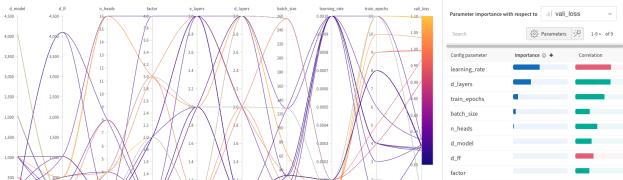
(c) Non-stationary transformer



(d) PatchTST



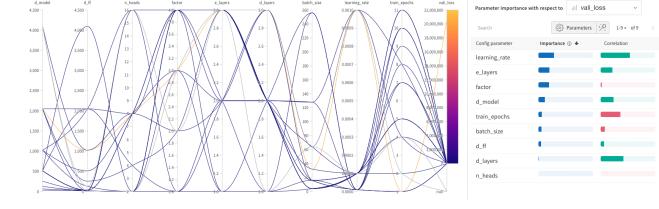
(e) Mamba



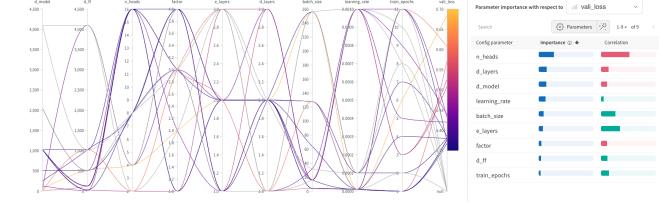
(f) TimeMixer

Fig. 5: Parallel coordinates plot on ETTh1 dataset

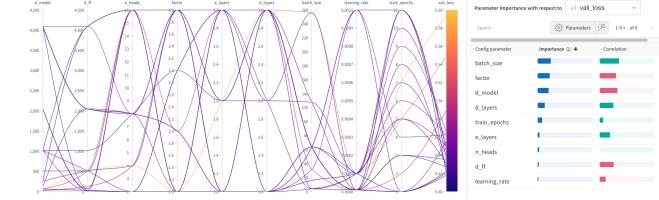
The tuning results highlight the significant influence of key hyperparameters such as d_model , learning rate, and batch size on model performance. Our pipeline, which leverages Ray Tune and Weights & Biases for scalable tuning and visualization, provides an efficient framework for integrating additional models. Future work will focus on expanding model coverage, exploring



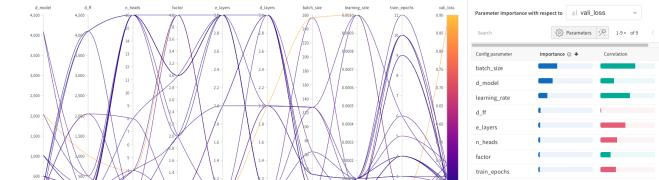
(a) Autoformer



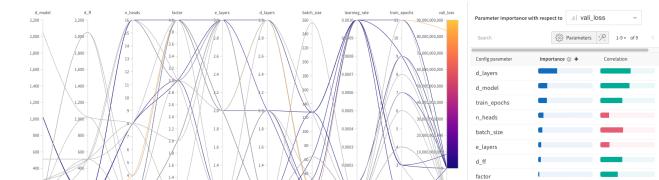
(b) Crossformer



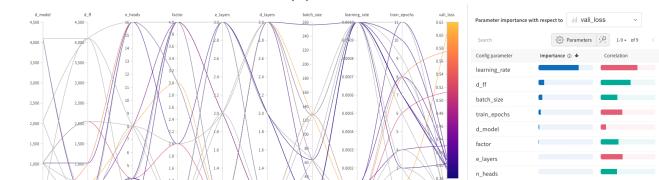
(c) Non-stationary transformer



(d) PatchTST



(e) Mamba



(f) TimeMixer

Fig. 6: Parallel coordinates plot on Weather dataset

advanced search techniques, and addressing out-of-memory (OOM) errors through distributed hyperparameter tuning across multiple GPUs on High Performance Computing (HPC). The code and results are publicly available to facilitate ongoing research in this area.

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