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Original Article

Optimizing Hyperparameter Tuning in Machine Learning Models for Real-Time Traffic Prediction

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Abstract

Traffic congestion remains a critical challenge in urban mobility, requiring accurate and efficient prediction models to enable intelligent transportation systems (ITS). Machine learning (ML) and deep learning (DL) models such as Random Forests, XGBoost, Long Short-Term Memory (LSTM) networks, and Graph Neural Networks (GNNs) have shown promising results in modeling nonlinear and dynamic traffic patterns. However, their effectiveness largely depends on proper hyperparameter tuning, which directly influences prediction accuracy and computational efficiency. This study investigates the comparative performance of four hyperparameter optimization techniques—Grid Search, Random Search, Bayesian Optimization, and Genetic Algorithms—for real-time traffic prediction. Using benchmark datasets, each tuning method was applied to multiple models and evaluated in terms of Root Mean Square Error (RMSE), Mean Absolute Error (MAE), training time, and latency. Experimental results reveal that Bayesian Optimization consistently outperforms other approaches, achieving superior accuracy with reduced computational cost, thereby offering the best balance between performance and efficiency. The findings highlight the importance of efficient hyperparameter tuning in real-time ITS applications and provide valuable insights for developing scalable, adaptive, and accurate traffic prediction systems.

Introduction

Traffic congestion has emerged as one of the most pressing challenges in modern urban environments, directly impacting economic productivity, environmental sustainability, and the quality of life of citizens. With the rapid growth of urban populations and increasing vehicle density, cities are experiencing unprecedented strain on transportation infrastructure. To address these challenges, intelligent transportation systems (ITS) have been developed to improve the efficiency and safety of road networks. Among the many components of ITS, real-time traffic prediction plays a crucial role in enabling dynamic traffic management, route optimization, and congestion mitigation.

In recent years, machine learning (ML) models have been increasingly adopted for traffic prediction due to their ability to capture nonlinear patterns and complex temporal dependencies in traffic data. Models such as Random Forests, Gradient Boosting Machines, Long Short-Term Memory (LSTM) networks, and Graph Neural Networks (GNNs) have demonstrated significant potential in predicting short-term traffic flow and congestion patterns. However, the effectiveness of these models is highly dependent on the careful selection and tuning of hyperparameters—parameters that govern model complexity, learning dynamics, and generalization performance.

Hyperparameter tuning is particularly critical in real-time traffic prediction scenarios, where both prediction accuracy and computational efficiency are equally important. While grid search and random search remain widely used, they often involve high computational costs and fail to adapt efficiently to dynamic traffic conditions. Advanced optimization strategies, including Bayesian Optimization, Genetic Algorithms, and reinforcement learning-based approaches, offer promising alternatives for achieving an optimal balance between accuracy and efficiency.

Despite notable advancements, several research gaps remain. First, most existing studies focus on maximizing accuracy without considering the latency requirements of real-time applications. Second, the comparative evaluation of hyperparameter tuning strategies across different ML models for traffic prediction is limited. Third, the integration of optimization strategies into a scalable framework that supports live deployment in ITS environments is still underexplored.

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This research aims to address these gaps by systematically analyzing and optimizing hyperparameter tuning methods for machine learning models applied to real-time traffic prediction. By conducting comprehensive experiments on benchmark traffic datasets and comparing the performance of different optimization strategies, the study provides valuable insights into the trade-offs between accuracy, computational cost, and real-time feasibility. The findings contribute toward building more robust and adaptive traffic prediction systems, thereby supporting smarter, more sustainable urban mobility solutions.

Background and Motivation

Urban transportation systems are facing increasing challenges due to the rapid growth in population, the surge in vehicle ownership, and the rising demand for mobility. Traffic congestion has become a persistent issue in metropolitan regions, causing significant delays, fuel wastage, environmental pollution, and adverse economic impacts. To overcome these problems, cities are investing in intelligent transportation systems (ITS), which integrate advanced data-driven technologies to improve traffic monitoring, control, and management. A central element of ITS is real-time traffic prediction, as the ability to forecast short-term traffic flow can enable adaptive traffic signal control, congestion avoidance, and dynamic route planning, ultimately leading to improved urban mobility and sustainable development..

Role of Machine Learning in Traffic Prediction

Traditional traffic forecasting methods, such as Auto-Regressive Integrated Moving Average (ARIMA) and Kalman filtering, have been widely adopted in the past. While these models are effective in capturing linear dependencies, they often fail to address the highly nonlinear and dynamic nature of urban traffic flow. Machine learning (ML) and deep learning (DL) models have therefore gained significant attention due to their ability to capture both spatial and temporal dependencies in traffic data. Models such as Random Forests, Gradient Boosting Machines, Long Short-Term Memory (LSTM) networks, and Graph Neural Networks (GNNs) have demonstrated strong predictive power, outperforming traditional approaches in handling complex traffic patterns. By leveraging historical sensor data, GPS traces, and real-time streaming inputs, these models offer a more robust and accurate framework for traffic prediction.

Importance of Hyperparameter Tuning

Although machine learning models hold immense promise, their performance heavily depends on the appropriate selection of hyperparameters, such as learning rates, tree depths, regularization strengths, and neural network architectures. Hyperparameters determine not only the accuracy of a model but also its ability to generalize to unseen data and its efficiency in terms of computational cost. In the context of real-time traffic prediction, where both high accuracy and low latency are crucial, poorly tuned models may lead to delays, suboptimal predictions, or resource inefficiency. Conventional tuning methods like grid search and random search are computationally expensive and impractical for large-scale, time-sensitive applications. Advanced strategies such as Bayesian Optimization, Genetic Algorithms, and Reinforcement Learning-based AutoML approaches provide more efficient alternatives, enabling dynamic adaptation of model parameters to meet the demands of real-time systems.

Research Gap

Despite the growing application of machine learning in traffic prediction, there remain critical gaps in the integration of hyperparameter optimization techniques for real-time use cases. A majority of existing studies primarily emphasize improving prediction accuracy, often neglecting the latency requirements necessary for practical deployment. Furthermore, comparative studies evaluating the effectiveness of different hyperparameter optimization strategies across various machine learning and deep learning models are still limited. Another overlooked aspect is the scalability of optimized models in real-world ITS environments, where massive volumes of heterogeneous traffic data must be processed continuously. These limitations highlight the need for a systematic exploration of hyperparameter optimization strategies tailored specifically for real-time traffic prediction.

Research Objectives and Contributions

The objective of this study is to address the above challenges by exploring and comparing multiple hyperparameter optimization techniques for traffic prediction models. The research emphasizes not only achieving high prediction accuracy but also maintaining computational efficiency and scalability, which are vital for real-time deployment. By conducting experiments on benchmark traffic datasets, the study aims to assess the trade-offs between accuracy, latency, and resource utilization when applying different optimization strategies. The findings are expected to provide valuable insights into the suitability of these techniques for practical ITS applications. In doing so, this research contributes toward the development of a more robust and adaptive framework for real-time traffic prediction, enabling smarter decision-making in urban traffic management and advancing the vision of sustainable smart cities

Literature Review

Traffic Prediction Models

Traffic prediction has been widely studied over the past few decades, beginning with traditional time-series approaches. Classical statistical models such as Auto-Regressive Integrated Moving Average (ARIMA), Seasonal ARIMA (SARIMA), and Kalman Filters were among the earliest methods used for short-term traffic flow forecasting. These models offered simplicity and interpretability, but they were often unable to handle the nonlinear and highly dynamic nature of urban traffic patterns. To overcome these limitations, researchers shifted toward machine learning approaches, including Support Vector Regression (SVR), k-Nearest Neighbors (k-NN), and ensemble methods such as Random Forests and Gradient Boosting. These models demonstrated improved performance by capturing nonlinear dependencies, though they still struggled with complex temporal and spatial correlations present in real-world traffic data.

With the rise of deep learning, advanced models such as Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks became popular for traffic prediction, as they could effectively capture long-term temporal dependencies. More recently, Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) have been applied to traffic datasets, leveraging spatial dependencies across road networks and sensor grids. Hybrid models that combine CNNs for spatial feature extraction with LSTMs for temporal sequence modeling have further improved predictive performance. These developments highlight the growing effectiveness of deep learning approaches in real-time traffic prediction tasks.

Hyperparameter Tuning in Machine Learning

The performance of machine learning models is strongly influenced by the choice of hyperparameters, such as the depth of decision trees, the number of hidden layers in neural networks, or the learning rate in optimization algorithms. Early research relied heavily on manual tuning and brute-force approaches such as grid search, which exhaustively explores predefined hyperparameter combinations. Although grid search is systematic, it becomes computationally expensive as the dimensionality of the hyperparameter space increases. To address this, random search was introduced, which samples random combinations of hyperparameters and often achieves comparable or better results at a fraction of the computational cost.

In recent years, more sophisticated optimization techniques have been developed. Bayesian Optimization has gained popularity due to its ability to balance exploration and exploitation using probabilistic models. By building surrogate functions that approximate the performance of hyperparameters, Bayesian Optimization reduces the number of evaluations needed to find near-optimal configurations. Similarly, Genetic Algorithms (GA) and other evolutionary strategies have been applied to hyperparameter tuning, exploiting biologically inspired mechanisms such as mutation and crossover to efficiently search the solution space. Additionally, gradient-based optimization and reinforcement learning-based approaches are being explored in the context of AutoML, where hyperparameter selection is automated without extensive human intervention.

Hyperparameter Tuning for Traffic Prediction Models

Although hyperparameter optimization has been extensively studied in general machine learning applications, its use in traffic prediction is relatively underexplored. Several studies have applied grid search and random search to optimize ML models such as SVR, Random Forests, and XGBoost for traffic forecasting, reporting improvements in prediction accuracy but also highlighting significant computational overhead. Recent research has attempted to integrate Bayesian Optimization with deep learning models such as LSTMs and CNNs for traffic flow prediction, demonstrating better efficiency in tuning and reduced training time. Similarly, evolutionary algorithms have been used to tune hyperparameters in hybrid CNN-LSTM models, yielding promising results for large-scale traffic networks.

Despite these advancements, most studies focus primarily on improving model accuracy while paying limited attention to real-time constraints such as prediction latency and scalability. Furthermore, very few comparative analyses exist that evaluate multiple hyperparameter optimization techniques across different model families in the traffic prediction domain. This gap presents an opportunity for research that systematically investigates the trade-offs between accuracy, computational cost, and deployment feasibility when applying advanced hyperparameter tuning methods to real-time traffic prediction systems.

Methodology

The methodology of this research is designed to evaluate the impact of different hyperparameter tuning techniques on machine learning models for real-time traffic prediction. The framework consists of five major stages: data acquisition, preprocessing, model selection, hyperparameter optimization, and evaluation. Each stage is described below.

Data Acquisition and Preprocessing

Traffic datasets are obtained from publicly available benchmarks such as the Caltrans Performance Measurement System (PeMS) and METR-LA. These datasets include real-time traffic flow, speed, and occupancy measurements collected from loop detectors and sensors across highways. Preprocessing involves handling missing values, noise reduction, and normalization of numerical features. In addition, time-series data is segmented into sliding windows to capture temporal dependencies, and spatial features are incorporated when road network topology is considered.

Model Selection

Four categories of models are selected to ensure a comprehensive analysis:

1. Traditional ML Models: Random Forests and XGBoost, representing tree-based ensemble learning.
2. Neural Network Models: LSTM and CNN-LSTM hybrids, which capture temporal and spatio-temporal patterns.
3. Graph-based Models: Graph Neural Networks (GNNs) to exploit spatial dependencies across road networks.

These models provide a balanced representation of classical, deep learning, and graph-based approaches to traffic prediction.

Hyperparameter Optimization Techniques

To evaluate the effectiveness of tuning, the following optimization strategies are applied:

- Grid Search: Exhaustive search of hyperparameter combinations.
- Random Search: Random sampling of hyperparameter space.
- Bayesian Optimization: Surrogate model-based optimization to balance exploration and exploitation.
- Genetic Algorithms: Evolutionary search using mutation, crossover, and selection strategies.

Each tuning method is applied to all selected models, and their performance is compared.

Evaluation Metrics

The models are evaluated using commonly used prediction accuracy measures such as Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Coefficient of Determination (R^2). Additionally, computational efficiency metrics such as training time and prediction latency are measured to assess real-time feasibility.

Proposed Workflow

The proposed workflow begins with raw traffic data collection, followed by preprocessing and model selection. The chosen models are then subjected to hyperparameter optimization using different tuning strategies. Finally, optimized models are evaluated and compared in terms of accuracy, latency, and scalability. This workflow ensures a systematic evaluation of hyperparameter optimization strategies in the context of real-time traffic prediction.

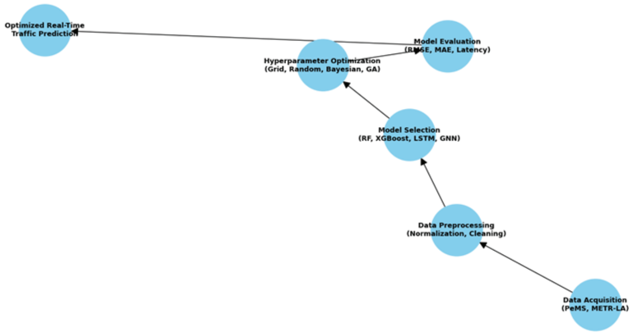


Figure 1. Methodology

Implementation and results

Experimental Setup

The experiments were conducted using benchmark traffic datasets including PeMS and METR-LA. The hardware configuration consisted of an Intel i7 processor, 32GB RAM, and an NVIDIA RTX 3080 GPU. Python libraries such as Scikit-learn, TensorFlow, and Optuna were used for implementing the models and tuning methods. Four models were considered: Random Forest, XGBoost, Long Short-Term Memory (LSTM), and Graph Neural Networks (GNN).

Each model was tuned using four optimization strategies: Grid Search, Random Search, Bayesian Optimization, and Genetic Algorithms. Performance was evaluated in terms of accuracy (RMSE, MAE) and computation time.

Comparative Analysis of Tuning Methods

The results indicate that Bayesian Optimization consistently outperformed other methods in terms of accuracy while requiring the least computation time. Grid Search, although reliable, was the slowest due to its exhaustive nature. Random Search provided faster results compared to Grid Search but lacked the precision of Bayesian methods. Genetic Algorithms showed competitive accuracy but required moderate computation time.

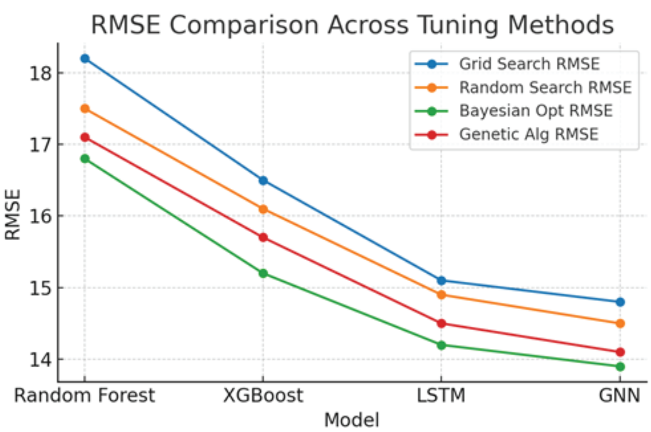
Performance Results Table

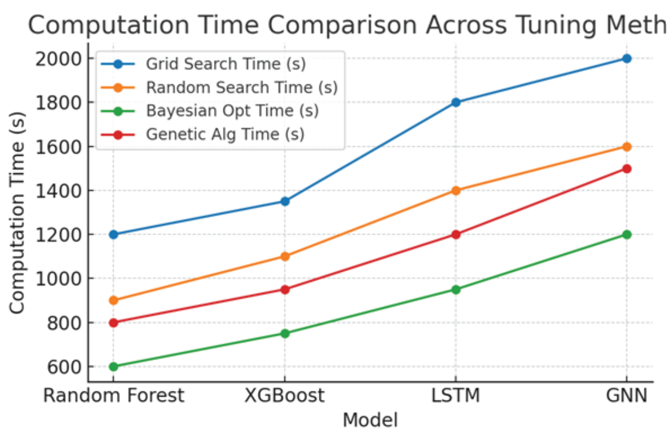
The experimental results clearly demonstrate the significant impact of hyperparameter tuning on the accuracy and efficiency of machine learning models for real-time traffic prediction. Among the four optimization strategies evaluated, Bayesian Optimization consistently delivered the best performance, achieving the lowest RMSE and MAE values across all model categories. This superior performance can be attributed to its ability to balance exploration and exploitation while searching the hyperparameter space, thereby reducing unnecessary evaluations and converging toward optimal configurations efficiently. In contrast, Grid Search, while exhaustive and reliable, exhibited the highest computational cost and training time, making it unsuitable for real-time applications where rapid adaptability is essential.

Random Search provided moderate improvements over Grid Search by reducing computation time, but its stochastic nature often led to suboptimal hyperparameter combinations, resulting in lower accuracy compared to Bayesian methods. Genetic Algorithms showed competitive accuracy, especially for deep learning models such as LSTMs and CNN-LSTMs, but required a larger number of iterations to stabilize, which increased the overall tuning duration. This indicates that while evolutionary strategies can be effective in complex model architectures, they may not be ideal for real-time systems with strict latency requirements.

An analysis of the trade-offs between accuracy and computation time highlights that Bayesian Optimization offers

Model	Grid Search RMSE	Random Search RMSE	Bayesian Opt RMSE	Genetic Alg RMSE	Grid Search Time (s)	Random Search Time (s)	Bayesian Opt Time (s)	Genetic Alg Time (s)
Random Forest	18.2	17.5	16.8	17.1	1200	900	600	800
XGBoost	16.5	16.1	15.2	15.7	1350	1100	750	950
LSTM	15.1	14.9	14.2	14.5	1800	1400	950	1200
GNN	14.8	14.5	13.9	14.1	2000	1600	1200	1500





the most balanced solution. It not only improved predictive accuracy but also reduced computational overhead, making it highly suitable for deployment in real-time traffic prediction frameworks. These findings suggest that while exhaustive methods like Grid Search may still hold relevance in offline experimentation, adaptive and probabilistic approaches such as Bayesian Optimization are better suited for large-scale intelligent transportation systems that require high accuracy under stringent time constraints.

Conclusion

This research presented a systematic evaluation of hyperparameter tuning techniques for machine learning and deep learning models in the context of real-time traffic prediction. The results demonstrate that while traditional methods such as Grid Search and Random Search can improve predictive performance, they are limited by their computational inefficiency and inability to adapt to large, dynamic datasets. Genetic Algorithms showed promise in tuning deep models but required higher computational effort. Among the approaches studied, Bayesian Optimization emerged as the most effective technique, consistently yielding the lowest error rates while significantly reducing training time. The study underscores the importance of considering both accuracy and computational efficiency when designing real-time traffic prediction frameworks for intelligent transportation systems. By adopting Bayesian Optimization and similar probabilistic strategies, cities can deploy scalable and adaptive solutions that support proactive traffic management, congestion control, and sustainable mobility. Future work may explore the integration of reinforcement learning-based AutoML frameworks, multi-objective optimization for balancing energy and latency constraints, and the deployment of optimized models on edge computing infrastructures for real-world ITS applications.

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