

Evaluating Machine Learning Models for PM2.5 Prediction: A Case Study on Air Pollution in Beijing

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ABSTRACT

Large pollution impacts on human, animal, and plant health, along with advanced computing technologies capable of managing big data, create new opportunities for applying ML to improve air quality observation. Questions also continue to increase as more are created about how the performance of newer, hybrid ML models is matched to a particular application for the most suitable ML model. This paper presents a systematic review of state-of-the-art studies that implement ML techniques in the context of PM2.5 concentration prediction, focusing on analyzing dataset size, hyperparameters, and preprocessing techniques to answer these questions. This review investigates some proposed ML techniques and models applied in Beijing by highlighting their main characteristics and relevant results. They then pointed out that hybrid models are capable of uncovering the hidden features of data, which was not possible by single approaches with high dimensions. Another conclusion was drawn that air pollution prediction models have to be compared under the same conditions with the same future characteristics.

Keywords: Air Pollution Prediction; Machine Learning Models; Comparative Analysis; Beijing; ANN



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1. Introduction

PM2.5 leads to a multitude of diseases, including respiratory, cardiovascular, and laryngeal cancers (D. R. Liu et al., 2020). High PM2.5 concentrations are the reason for the deaths of around 1.6 million every year in China alone (He & Christakos, 2018). The environmental effects of total and partial pollutants are severe problems that have directly or indirectly harmed human, animal, and plant health. However, the reduction in the risk of pollution can be translated into reducing economic costs and maintaining human lives due to stroke, lung cancer, and chronic and acute respiratory diseases. In this context, several predictive models were proposed by researchers to support environmental management and prevent accidents. One of the most important areas of research involves using appropriate tools and mathematical models to analyze environmental data and obtain accurate pollutant concentration forecasts.

In general, two main types of models are applied in this domain: statistical and machine learning models (ML) (Du et al., 2022a). The statistical models include examples like ARIMA (D. J. Liu & Li, 2015), regression (F. Jiang et al., 2021), grey models (Wu et al., 2017), and SVM (Xu et al., 2017). Most of these models present very good results. For example, SVM has been popularly applied to forecast studies owing to its exceptional performance in solving nonlinear problems as indicated by Xu et al. (2017). On the contrary, ML refers to a field of artificial intelligence that enables machines with capabilities of learning based on a set of algorithms that handle data for prediction purposes. Deep learning is a subbranch of machine learning and the highest in artificial intelligence. It involves designing machines that learn and perform as humans would by replicating the functions of the human brain's neurons and neural networks. From the papers reviewed, several single models and techniques have been combined to form hybrids or ensemble models to outperform. This is to overcome specific issues faced by the single model's face. (Zhang et al., 2018) categorized hybrid models into three types including (Simple hybrid models, Hybrid models with preprocessing methods, and Intelligent hybrid models).

Both hybrid and ensemble models are techniques that try to enhance the performance of predictive models by their different methods, though both differ in their approach and implementation. Results from the reviewed articles confirm the fact that generally, hybrid and ensemble models outperform single models. In the study of (Zhang et al., 2018), for example, it was concluded that "ensemble models perform significantly better than the single best model in stock price forecasting". Similarly, (Wang et al., 2020) found that the hybrid model assembling deep learning with traditional machine learning techniques outperformed single models in air quality prediction. These results concluded that the combination of strengths from several models can lead to more accurate predictions. They are often used to reduce the impact of individual model errors and improve the stability of the predictions.

The goal of a hybrid model is to leverage the strengths of different approaches to compensate for their weaknesses, leading to a more accurate and robust model (Kai et al., 2017). Hybrid models combine multiple algorithms or techniques within a single model to improve accuracy. For example, a hybrid recommendation system may combine collaborative filtering and content-based filtering techniques to make recommendations (Bach et al., 2016). While some researchers use an ensemble model when one model is not enough to learn the problem's complexity, or various models make different mistakes that are corrected after combining, on the other hand, an ensemble model will combine several models' predictions to come up with a single and better forecast. According to (Shahriari et al., 2020), the common ensemble techniques include bagging, boosting, and stacking as mentioned by Ji & Levinson, 2020.

Thus, while hybrid models combine several approaches within one model, in ensemble models, several models are combined to produce a more accurate prediction. Both techniques have strengths and weaknesses and can be used depending on the problem. Furthermore, there is another type of AI model called the meta-learning model. Meta-learning is a type of machine learning that deals with designing and applying algorithms that can learn from previous learning experiences (Noguer et al., 2021). Meta-learning models can learn to adapt to new tasks and data sets based on their previous experience. This makes them particularly useful in scenarios where data is limited or when new data sets are constantly coming in. With more advanced and sophisticated machine learning models being developed and tested, the performance and accuracy of the models continue to improve. This improvement is because these models can capture more complex patterns and relationships in the data, resulting in better predictions and recommendations. The incorporation of hybrid, ensemble, and meta-learning models, which combine multiple models to leverage their strengths, has also improved performance in many cases (Neshat et al., 2021).

Other characteristics of geographic location, meteorological, forecast horizon, and temporal features are only some of the factors that may arise when comparing the above-mentioned prediction models for different geographic locations. These external factors play a great role in determining the accuracy of the predictions (F. Jiang et al., 2021). Each of them needs to be considered separately. For example, the paper (F. Jiang et al., 2021) noticed that PM2.5 characteristics may have hourly, daily, and monthly variations. Lower concentrations were seen in early morning and evening than at noon and late night because of the sun effect. The daily activities may be different depending on the day of the week, where higher concentrations were seen on Wednesdays, Fridays, and Sundays than the concentration in the other days. Besides, regarding the season, winter has a larger PM2.5 concentration than in spring and summer.

According to recent studies, this research will answer the following research questions (RQ):

RQ1: Is it possible to compare the accuracy of machine learning prediction models for PM2.5 levels across different geographic locations over a long-term period?

RQ2: How do machine learning models compare in predicting PM2.5 levels in the same geographic location across different time periods (monthly, seasonal, yearly), over a three-year dataset?

RQ3: What model, using a six-month sample period and keeping everything constant such as area and date for PM2.5 forecasting with short-term daily data input gives the best result?

The present work tends to give an overview of the current AI-based PM2.5 prediction models in Beijing, China. Beijing is the capital city of the People's Republic of China, lying in the northern part of the country. It hosts more than 21 million people and is one of the most populous cities in China. In the last couple of years, Beijing has been suffering from severe air pollution problems, especially about PM2.5, which is harmful to human health. Because of that, the government has taken several measures, such as the establishment of strict air quality standards, investment in clean energy technologies, and encouragement of public transportation, to reduce air pollution. However, despite those measures, the PM2.5 pollution remains a big problem in Beijing, and scholars have developed some AI-based PM2.5 prediction models to learn more about and manage the issue.

2. Literature Review

The literature review section of this paper offers a comprehensive exploration of existing research on air pollution, with a focus on key pollutants and their implications, assessment of the performance of employed machine learning models, and scrutiny of the hyperparameter tuning strategies employed. This general review will start with some models conducted in Beijing. In This general review will be initiated with some models conducted in Beijing. In Feng (Feng et al., 2015), data ranging from September 2013 to October 2014 is used. The dataset contains meteorological data and pollutant concentrations such as PM2.5, PM10, NO2, SO2, O3, CO. A backpropagation neural network - BP - compared to models that incorporate trajectory and wavelet transformation. The results showed that the addition of trajectory and wavelet transformation enhanced the model performance for RMSE. For instance, the RMSE of 1 day using BP alone was 28.63, while for BP + trajectory model + wavelet, the RMSE reduced to 15.65.

In paper, P. Jiang (P. Jiang et al., 2019), they use only air pollutants, PM2.5, SO2, NO2, CO, and O3, found a better RMSE using ICEEMDAN as a decomposition tool and the prediction model ICA-BPNN. The dataset used in this study covers from November 2016 to July 2017. Comparative work has been carried out for several models to prove the superiority of the proposed model: ARIMA, GRNN, and several kinds of neural networks, including BPNN, SBO-BPNN, ICA-BPNN, and ICEEMDAN-ICA-BPNN. They found that the best results belonged to the ICEEMDAN-ICA-BPNN model with RMSE of 1.8902 and R^2 of 0.9955. The input with air pollutants of humidity, PM10, SO2, NO2, O3, and CO has been utilized in Sun & Li 2020. Further, several models are compared in the study like BPNN, IBPNN, ELM, LSSVR, and stacking, while PACF+SCC + BPNN+IBPNN+ELM has given a minimum RMSE 3.15 and a maximum R^2 value of 0.999 for stacking model.

F. Jiang (F. Jiang et al., 2021) considered the dataset of a number of meteorological factors, including wind speed, wind direction, temperature, precipitation, pressure, relative humidity, and pollutant concentrations: PM2.5, PM10, NO2, SO2, O3, CO. The performances of several models were compared, including linear regression (LR), autoregressive integrated moving average (ARIMA), support vector regression (SVR), backpropagation neural network (BPNN), long short-term memory (LSTM), gated recurrent unit (GRU), deep temporal convolutional neural network (DeepTCN), and other models that use decomposition methods. The minimum RMSE for one hidden was obtained by CEEMDAN + SVR with 1.2813, followed by CEEMDAN + LSTM with 1.2892 and CEEMDAN + DeepTCN with 1.1064.

Du (Du et al., 2022a) presented the TVF-EMD-HHO-ELM model, which was compared with several models such as Persistence model, TVF-EMD-ELM, VMD-HHO-ELM, ICEEMDAN-HHO-ELM, TVF-EMD-SCA-ELM, and TVF-EMD-HHO-ELM, using data ranging from April 1, 2018, to August 10, 2019, for PM2.5 only. The scores for RMSE and R^2 , in order, were: 18.2972, 0.4654, 14.5847, 0.8883, 5.7581, 0.9721, 5.4582, 0.9524, 1.8169, 0.9965, 0.9442, 0.9986.

On the other hand, Yang & Zhang (Yang & Zhang, 2023) suggested an attention mechanism for prediction model ADST-ML (CNN+LSTM), which they put to a test against HA, Regression, ARIMA, Random forest, MLP, LSTM, LSTM-FC with individual results of RMS for 1 hour ahead prediction were: 56.866, 38.815, 36.235, 48.663, 27.534, 28.732, and 19.454, respectively on PM2.5 and meteorological data of May 2014 to April 2015; the learning rate was 0.0009 reported an RMSE of 10.974 while for window size 12 an RMSE of 15.374 reported.

Al-qaness (Al-qaness et al., 2023) updated the Informer model using deep learning with ResInformerStack and present a comparison between the results obtained from the data between January 1, 2014, and February 17, 2022, using the models InformerStack and ResInformer. It showed that the proposed model is superior to the other models. Results for RMSE and R^2 : (0.2852, 0.8285), (0.2692, 0.8472), (0.2822, 0.8320), and (0.2623, 0.8549). Table 1 summarizes the literature studies models and their performance.

Table 1. A summary of the literature studies models and their performance.

Author	Method	Dataset	Period	Performance Metrics (RMSE/R ²)
Feng et al. (2015)	Backpropagation Neural Network (BP) + Trajectory + Wavelet	September 2013 - October 2014	1 Year	RMSE from 28.63 to 15.65
P. Jiang et al. (2019)	ICEEMDAN-ICA-BPNN	November 2016 - July 2017	9 Months	RMSE= 1.8902, R ² =0.9955
Sun & Li (2020)	Stacking Model (PACF+ SCC+BPNN+IBPNN+ELM)	Humidity and Air Pollutants (PM10, SO2, NO2, O3, CO)	January 1, 2017, to January 25, 2017	RMSE= 3.15, R ² =0.999
F. Jiang et al. (2021)	CEEMDAN + SVR, CEEMDAN + LSTM, CEEMDAN + DeepTCN	Meteorological and Pollutant Data (PM2.5, PM10, NO2, SO2, O3, CO)	2 January 2015 to 31 December 2017	RMSE from 1.2813 to 1.1064
Du et al. (2022a)	TVF-EMD-HHO-ELM	April 1, 2018 - August 10, 2019 (PM2.5)	1st April 2018 to 10th August 2019	RMSE= 0.9442, R ² =0.9986
Yang & Zhang (2023)	ADST-ML (CNN + LSTM)	May 2014 - April 2015	1 Year	RMSE= 10.974,
Al-qaness et al. (2023)	ResInformerStack	January 1, 2014 - February 17, 2022	8 Years	RMSE= 0.2623, R ² =0.8549

3. Results and Discussion

This section will present a summary of findings and answers the research questions. This paper reviewed the state-of-the-art ML techniques applied for PM2.5 concentration prediction using a case study with datasets from Beijing. Many Machines Learning (ML) models were discussed, which included, but were not limited to, schemes such as BPNN, SVR, advanced hybrid schemes of CEEMDAN-LSTM, and ResInformerStack. From this review, it became obvious that important methods for improvement included those for data preprocessing and tuning of hyperparameters, alongside using big dataset sizes. This section will discuss the findings of this study based on a comparative analysis of the different air pollution prediction models.

3.1. Literature Survey Analysis

This section presents the importance of deploying the literature of recent studies to identify the key important of used methods and features of each of them. The word cloud depicted a number of different methods and techniques adopted in research for air pollution prediction from 2010 to 2025. It also showed that the size of each word is directly proportional to the usage and role it has played in PM2.5 prediction. Figure 1 shows the Word cloud analysis of implementing methods.

- Best Model

The word cloud diagram shows the importance of different methods with their respective values of RMSE. It reflects the trend in predictive models from simple neural networks toward hybrid complex architectures. The earlier methods, like BP, give higher values of RMSE, which reflect poor predictions. In contrast, some of the recent methods are ResInformerStack (Al-qaness et al., 2023) with the lowest RMSE of 0.2623, reflecting the highest accuracy of prediction. The second-best model was that by Du et al. (2022a), which proposed TVF-EMD-HHO-ELM with an RMSE of 0.9442. The diagram also shows a growing trend for the use of combinations like ICEEMDAN-ICA-BPNN and CEEMDAN + SVR + LSTM to enhance performance. This constitutes a logical step in the direction toward the goal, which is that of minimizing error rates by incorporating ensemble models, wavelet transforms, and deep learning methods. Among these, ResInformerStack has the lowest RMSE, indicating the state-of-the-art in time-series

forecasting. Overall, the increasing complexity and sophistication of the models over time underline the continuous effort in improving forecasting accuracy through method innovations.

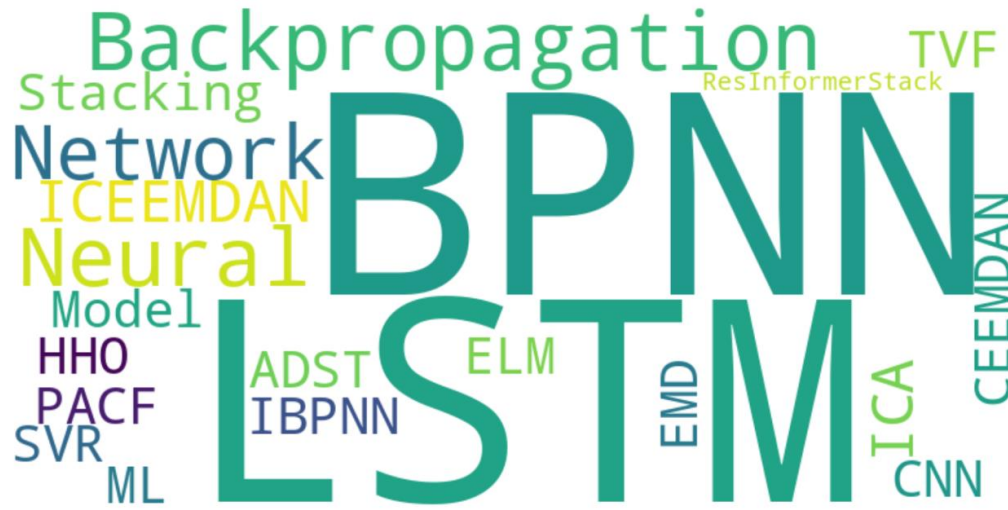


Figure 1. A Word Cloud analysis of implementing methods

- **Hybrid Models**

Hybrid models such as CEEMDAN + LSTM, TVF-EMD-HHO-ELM, and ResInformerStack are some of the most preferred models. These hybrid models are more accurate since they can handle noisy and nonlinear data. Hybrid models tend to outperform traditional ones because they have the capability to capture time-series variations and extract hidden patterns from high-dimensional data. They also eliminate noise by using decomposition techniques such as CEEMDAN and ICEEMDAN.

- **Duration of implementing datasets and methods**

Figure 2 shows heatmap diagram illustrates the duration of implementing datasets based on authors and methods used. Analysis and Major Information Provided by Heatmap of Dataset Duration by Method and Author

The Figure shows a heat map visualization of the dataset duration in years for various proposed methods of air pollution prediction by different authors during the years 2015-2023. The duration is color-mapped, with the darker shades showing longer durations. Longer datasets, like the 8-year dataset Al-Qaness et al. (2023) used, usually lead to better long-term predictions by capturing more historical trends and seasonal variations in air pollution levels. Even short-term datasets, such as Sun & Li (2020), can achieve very high accuracy based on advanced pre-processing and hybrid model approaches using stacking and decomposition. Although their dataset was for only 25 days, their model showed good performance, indicating the efficiency of stacking multiple models. P. Jiang et al. (2019) used a 9-month dataset for the ICEEMDAN-ICA-BPNN method, achieving high accuracy despite the short timeframe. It would further mean that the ICEEMDAN decomposition technique could be potent in handling short-term data, and it holds great potential to extract features meaningfully from minimal data. Overall, the models based on CEEMDAN performed impressively for a reasonable number of dataset durations. This may prove that the decomposition using techniques like CEEMDAN can enhance accuracy and robustness in air pollutant prediction models, which lack highly extensive datasets.

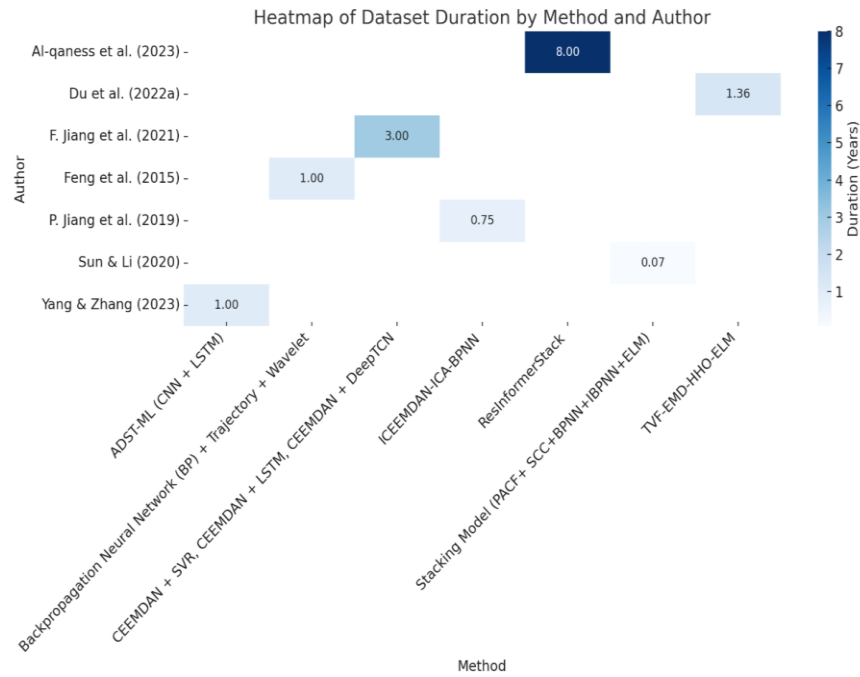


Figure 2. A heatmap diagram illustrates the duration of implementing datasets and methods

Figure 3 shows that the RMSE of the different methods in air pollution prediction is represented as a heatmap. The low value of RMSE reflects a high accuracy of prediction. The minimum RMSE, 0.2623, was obtained using the ResInformerStack method, which outperformed the other methods. The BP method has a maximum RMSE, 28.63, which is very high compared to hybrid models.

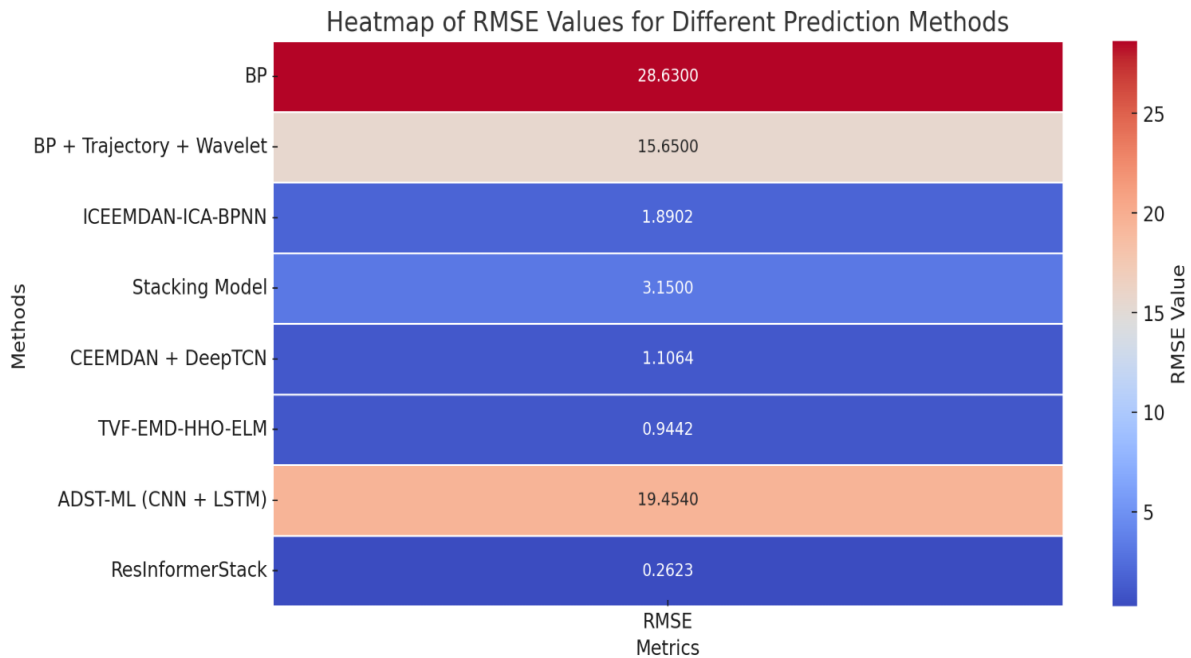


Figure 3. Heatmap diagram of the RMSE of the different methods

3.2. Answers to the Research Questions

- **RQ1: Whether the accuracy of machine learning prediction models for the PM2.5 long-term period could be compared for different geographic locations?**

Yes, the accuracy of machine learning prediction models across different geographic locations could be compared over a long period. However, the performance of each model will vary because of different climatic conditions, data availability, and input variables including meteorological factors and pollutant concentrations. Feng et al. (2015) and Du et al. (2022a) present that models with data preprocessing methods such as wavelet transformation and decomposition techniques like CEEMDAN and ICEEMDAN tend to perform better across different locations by reducing noise in long-term datasets. For instance, P. Jiang et al. (2019) represented the value of RMSE as 1.8902 for the ICEEMDAN-ICA-BPNN model in PM2.5 prediction of different areas. This showed that the advanced hybrid models can fit various geographic conditions with a high degree of accuracy in prediction. However, each model's performance should be validated using diverse datasets from different geographical locations to ensure generalizability.

- **RQ2: How do the machine learning models compare in the prediction of PM2.5 levels at the same location but across time periods, monthly, seasonal, and yearly, over a three-year dataset?**

Machine learning models present different performances when predicting PM2.5 at different time frequencies in the same location. Let's take F. Jiang et al. (2021) made a comparison between several models: CEEMDAN + SVR, CEEMDAN + LSTM, and CEEMDAN + DeepTCN using data over a period of three years. They generally found that all the decomposition techniques, like CEEMDAN, generally outperform the traditional models such as ARIMA and SVR on capturing seasonal and yearly variations with as low an error as 1.1064 RMSE. This means that the short-term models are LSTM sensitive to seasonal fluctuations, while the long-term models can catch yearly trends. In general, hybrid models with feature decomposition and recurrent neural networks provide better accuracy across different time horizons.

- **RQ3: Which model provides the best outcome for PM2.5 forecasting with a six-month sample period using the same area and date with short-term daily data input?**

From the reviewed studies, TVF-EMD-HHO-ELM model by Du et al. (2022a) and ResInformerStack model by Al-Qaness et al. (2023) had the superior performance of short-term PM2.5 forecasting with a daily data input. Du et al. (2022a) realized an RMSE of 0.9442 for the TVF-EMD-HHO-ELM model over six months, outperforming other models such as ICEEMDAN-HHO-ELM and VMD-HHO-ELM. Similarly, Al-Qaness et al. (2023) have shown that ResInformerStack has the best results for short-term predictions with an RMSE of 0.2623. The results reflect that hybrid models with decomposition techniques and deep learning frameworks have better accuracy for short-term PM2.5 forecasting.

4. CONCLUSION

This paper reviewed state-of-the-art ML techniques applied for PM2.5 concentration prediction using a case study with datasets from Beijing. The authors discussed many ML models, including but not limited to schemes such as BPNN, SVR, advanced hybrid schemes of CEEMDAN-LSTM, and ResInformerStack. From this review, it was clear that some of the important methods for improvements included data preprocessing, tuning of hyperparameters, and big dataset size usage. In this section, a discussion is done on the results of this study based on a comparative analysis between various models of air pollution prediction. First, let me give my opinion that hybrid model performances are superior to the traditional techniques of capturing high-dimensional data in order to come up with hidden patterns. The comparison analysis among the different models of air pollution prediction underlines the necessity of establishing similar conditions when considering time frames and datasets in order to provide the right evaluation. Results are explained in detail with the aim of responding to the research questions put forward in this work, illustrating the most performant models, and their usage for estimating air quality.

The word cloud depicted the sets of different methodologies and techniques adopted within the research in air pollution prediction throughout 2010 to 2025. The size of each word is directly proportional to the usage and the role it has played in PM2.5 prediction.

The word cloud diagram depicts the importance of various methods with their respective values of RMSE. It reflects the trend in predictive models from simple neural networks toward hybrid complex architecture. All the earlier methods, such as BP, provide higher values of RMSE, reflecting poor predictions. In contrast, some of the recent methods include ResInformerStack (Al-Qaness et al., 2023), and TVF-EMD-HHO-ELM (Du et al., 2022a), with far lower RMSE values of 0.2623 and 0.9442, respectively, hence showing their better performance. This diagram also

presents a growing trend in the usage of Hybrid models such as ICEEMDAN-ICA-BPNN and CEEMDAN + SVR + LSTM and TVF-EMD-HHO-ELM to boost performance. These hybrid models are more accurate since they can handle noisy and nonlinear data. The hybrid models outperform traditional models because they are capable of capturing time-series variations and extracting hidden patterns from high-dimensional data. Also, they remove noise by applying decomposition techniques like CEEMDAN and ICEEMDAN. The study also successfully answered the research question presented.

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