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## Short-term PM<sub>2.5</sub> forecasting using a unique ensemble technique for proactive environmental management initiatives

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Particulate matter with a diameter of 2.5 microns or less (PM<sub>2.5</sub>) is a significant type of air pollution that affects human health due to its ability to persist in the atmosphere and penetrate the respiratory system. Accurate forecasting of particulate matter is crucial for the healthcare sector of any country. To achieve this, in the current work, a new time series ensemble approach is proposed based on various linear (autoregressive, simple exponential smoothing, autoregressive moving average, and theta) and nonlinear (nonparametric autoregressive and neural network autoregressive) models. Three ensemble models are also developed, each employing distinct weighting strategies: equal distribution of weight among all single models (ESME), weight assignment based on training average accuracy errors (ESMT), and weight assignment based on validation mean accuracy measures (ESMV). This technique was applied to daily PM<sub>2.5</sub> concentration data from 1 January 2019, to 31 May 2023, in Pakistan's main cities, including Lahore, Karachi, Peshawar, and Islamabad, to forecast short-term PM<sub>2.5</sub> concentrations. When compared to other models, the best ensemble model (ESMV) demonstrated mean errors ranging from 3.60% to 25.79% in Islamabad, 0.81%-13.52% in Lahore, 1.08%-7.06% in Karachi, and 1.09%-12.11% in Peshawar. These results indicate that the proposed ensemble approach is more efficient and accurate for short-term PM<sub>2.5</sub> forecasting than existing models. Furthermore, using the best ensemble model, a forecast was made for the next 15 days (June 1 to 15 June 2023). The forecast showed that in Lahore, the highest PM<sub>2.5</sub> value (236.00  $\mu g/m^3$ ) was observed on 8 June 2023. Other days also displayed higher and poor air quality throughout the 15 days. Conversely, Karachi experienced moderate PM<sub>2.5</sub> concentration levels between 50  $\mu g/m^3$  and 80  $\mu g/m^3$ . In Peshawar, the PM<sub>2.5</sub> concentration levels were consistently unhealthy, with the highest peak (153.00  $\mu g/m^3$ ) observed on 9 June 2023. This forecasting experience can assist environmental monitoring organizations in implementing cost-effective planning to minimize air pollution.

#### KEYWORDS

air pollution, concentration, short-term PM 2.5 forecasting, single time series models, ensemble time series models, sustainable development, early warning system, decision making

## **1** Introduction

Maintaining a healthy atmosphere is vital for both humans and other living creatures. Air quality refers to the absence of harmful pollutants in the air. However, there are several deadly and fatal contaminants in the air nowadays, including PM2.5, nitrogen dioxides (NO<sub>2</sub>), carbon monoxides (CO), sulfur dioxides (SO<sub>2</sub>), ozone (O<sub>3</sub>), and PM<sub>10</sub> are the most hazardous pollutants, and these and several more contaminants cause air pollution (Donahue, 2018; Quispe et al., 2024; Yin et al., 2023; Shang and Luo, 2021). Currently, air pollution is increasing rapidly due to urbanization, industrialization, and overcrowding, and this leads to a significant increase in respiratory problems, premature birth, premature death, and lung disease, which cause death. The World Health Organization estimates that air contamination claims the lives of about ten million people each year. As discussed above, air pollutants contribute significantly to air quality degradation and affect human health and the environment due to increased industrial and human activity and the continuous use of fossil fuels (Manisalidis et al., 2020; Luo et al., 2024; Qiu et al., 2024; Shang et al., 2023). Currently, air pollution is Pakistan's most significant and alarming challenge, continuously being mentioned by social media and other platforms. This air pollution in Pakistan causes different health-related problems, mainly cardiac and respiratory. Thus, particular actions must be taken to prevent or reduce air pollution (Ullah et al., 2021; Iftikhar et al., 2024c; Du and Wang, 2013; Chen et al., 2024).

In the past, many researchers have developed solutions to this problematic air pollution issue. In this context, many researchers have applied classical regression, time series, machine learning, and hybrid models to find the optimum solution according to the nature of the data (Zhan et al., 2017; Xu et al., 2018; Abdullah et al., 2019; Dutta and Jinsart, 2021). For instance, the work (Geetha and Prasika, 2019) provides an LSTM in addition to two conventional forecasting models for estimating the levels of air pollutants (NO<sub>2</sub>, NOx, CO, SO<sub>2</sub>, O3, PM2.5, and PM10) in metropolises. The outcomes demonstrated that LSTM outperformed LR and ARIMA. Zaman et al. (2024) attempt intends to create machine learning models that are computationally efficient and simpler than those found in earlier studies. Findings indicated that the RF methodology performed marginally better than the XG-Boost and SVR techniques. In another research work, Zaman et al. (2021) predict PM2.5 concentrations throughout Malaysia by utilizing satellite-based AOD data to drive machine learning (ML) models such as (RF) and (SVR). Seven models were created for  $PM_{2.5}$  prediction. The testing analysis shows that the RF framework (R2 = 0.53-0.76) performs somewhat superior to SVR. On the other hand, using the most recent data on diseases and smog degree of severity, this study (Chen et al., 2017) designed an ANN-based model to forecast health hazards associated with smog. The outcomes demonstrated that empirical insights can aid researchers in getting the nonlinear correlations between the health risk the following day and present-day smog observations.

This work (Freeman et al., 2018), a forecast model for ozone levels averaged over 8 hours, was trained using novel deep learning techniques. A new technique for imputation was used to replace missing data and outliers in the collected data set. This method produced computed values based on the time and season closer to

the predicted value. (Carbo-Bustinza et al., 2023). Using a comparison of numerous hybrid varieties of time series models, this work extensively studies projecting ozone concentrations. According to the study, the suggested models perform noticeably superior to the standard models that were considered. However, this research (Xie et al., 2021) aims to apply the Hausdorff distance method to huge data to improve future cyclone effect predictions (Rakholia et al., 2023). Analyzed to develop a multi-step-ahead with multi-output type multivariate statistical model (NBEATS) to estimate the air quality with the auxiliary information. The data set was collected from six healthcare air quality centers in Vietnam. To compare the results and efficiency with the existing model, accuracy indices such as MAPE and RMSE were used. The result indicated that the developed (d-BEATS) multi-dimensional covariate model outperforms the existing models. In the work Bhatti et al. (2021), the researcher conducted a comparative study to estimate the air quality index for Pakistan. They used the SARIMA and factor analysis approaches to achieve this end. The study found that the SARIMA model outperforms others in attaining better estimation accuracy for Pakistan's air quality index. In another work, Ashraf et al. (2022) conducted an analysis based on the comparative study of machine learning and classical forecasting models to forecast air pollution data. This article uses the metrics, i.e., RMSE, MAE, and MAPE, to compare the classical and traditional models. The study suggested that the machine learning model performed more efficiently than the existing time series methods.

In the same way, Lin et al. (2019) performed an analysis based on machine learning and integrated assimilation data techniques to expand the air quality prediction for the Netherlands. The findings disclosed that the developed approach, which incorporates datadriven machine learning and a physics-based model, significantly improved the air quality forecast statistically. However, Kleine Deters et al. (2017) modeled PM25 urban pollution (Cotocollao and Belisario) using machine learning techniques. Based on the proposed machine learning model concentrations of PM2.5, the classifier accurately predicted PM2.5. Moreover, it was also observed that regression highlights better prediction when there are extreme conditions in the climate. This article shows that statistical approaches to machine learning techniques are relevant and significant in modeling PM2.5. Also, Borse (2020) highlighted the systematic review based on different statistical and machine learning techniques to forecast air quality. This systematic review concludes that data mining and machine learning approaches are highly used in forecasting and predicting air pollution. In another research, the author in Liu et al. (2020) analyzed the air quality index using machine learning algorithms. In this research work, the authors developed a novel machine-learning model based on the LSTM method and compared it with existing models. The results indicated that the developed model outputs were superior to the existing machine learning models in forecasting PM2.5. Garg and Jindal (2021) conducted a comparative study between machine learning and classical time series models to estimate PM2 5. The study found that the LSTM model outputs better and superior accuracy than the existing approaches. However, Ameer et al. (2019) conducted a comparative analysis based on advanced regression methods to predict the air quality index of smart cities. This article used RMSE and MAE to evaluate the

underlying models. The study found that the random forest model outperformed the existing methods.

On the other hand, Wang et al. (2019) proposed a hybrid model for air quality variables forecasting. This proposed method is a hybridization of the Long Short-Term Memory Neural Network and Gated Recurrent Unit (LSTM and GRU), an enhancement of ordinary LSTM. This work uses the data set of 74 cities in China for a comparative study. The outcomes disclosed that the proposed hybrid model outperformed the existing approaches. In the same way, Ejohwomu et al. (2022) conducted a comprehensive study to model the PM2.5 using hybrid machine learning methods. The finding showed that the hybrid machine-learning model outperformed the existing techniques. Also, Bai et al. (2019) for forecasting the hourly PM2.5 concentration, an ensemble neural network (E-LSTM) is proposed. The results show that the E-LSTM model, which comprises multiple LSTMs in different modes, outperforms the single LSTM regarding MAPE, RMSE, and correlation. Thus, different authors used various methods and models to find the optimum solution according to the nature of the data.

In contrast to the research mentioned earlier, this study introduces a comparatively simple and easily implemented new time series ensemble technique based on various linear (autoregressive, simple exponential smoothing, autoregressive moving average, and theta) and nonlinear (nonparametric autoregressive and neural network autoregressive) models to accurately and efficiently forecast short-term PM2.5 concentration in highly populated cities of Pakistan, including Lahore, Peshawar, Karachi, and Islamabad. Three ensemble models are developed, each using different weighting strategies: equal distribution of weight among all single models (ESME), weight assignment based on training average accuracy errors (ESMT), and weight assignment based on validation mean accuracy measures (ESMV). In this proposed time series ensemble approach, the PM<sub>2.5</sub> time series is first preprocessed by addressing missing values, stabilizing variance, ensuring normality, considering deterministic features, and addressing stationarity concerns. Then, six single time series and three ensemble models are used to forecast the preprocessed PM2.5 concentration time series. Six different accuracy metrics-the Diebold and Mariano tests and the correlation plot-are employed to assess the performance of this novel time series ensemble forecasting approach. The main contribution of this study is evaluating the performance of different single time series models and their proposed three novel ensemble models within the time series forecasting approach. The short-term forecasting performance for a whole year for air pollution (PM2.5) is evaluated, and the significance analysis of the differences in prediction accuracy is also investigated. To confirm the performance of the proposed time series ensemble technique, six different average accuracy metrics, an equal forecast statistical test, and a graphical assessment are used for comparison. This methodological proposal applies to the environmental management system to mitigate ozone pollution and is aimed at the stakeholders of the national air quality program. Unlike previous studies, which have been conducted from various perspectives globally, this analysis uses ensemble time series modeling and forecasting for short-term PM<sub>2.5</sub> levels in the Pakistan megacities. Finally, this approach could be extended to other cities in Pakistan and worldwide.

# 2 The proposed time series ensemble forecasting technique

This section elucidates the proposed time series ensemble technique for short-term (one-day-ahead)  $PM_{2.5}$  concentration forecasting in the megacities of Pakistan. In the proposed time series ensemble technique, the  $PM_{2.5}$  time series is first preprocessed by missing value, variance stabilization, and stationary concerns. Second, six different single time series models: the autoregressive, the simple exponential smoothing, the autoregressive moving averages, the theta, the nonlinear autoregressive, and the neural network autoregressive, and also three proposed ensemble models anticipate the cleaned  $PM_{2.5}$  concentration time series. The details about these steps are in the following subsections.

## 2.1 Preparation of raw data

This work uses daily PM2.5 concentration datasets from four monitoring megacities in Pakistan, Islamabad, Lahore, Karachi, and Peshawar, for five consecutive years: 2019, 2020, 2021, 2022, and 2023, respectively. Before starting modeling and estimating a time series of data, it should make sense to prepare the data. The goal of preprocessing is usually to simplify the modeling of the database. The PM<sub>2.5</sub> concentration time series case involves missing values, high volatility, a nonconstant mean, a long-run secular trend component, and specific seasonality. To achieve these, we first treated the missing values using the multivariate imputation by chained equations (MICE) method (Van Buuren and Oudshoorn, 2011; Zhou et al., 2023). The MICE is a robust, informative method of dealing with missing data in datasets. The procedure imputes missing data in a dataset through an iterative series of predictive models. In each iteration, each specified variable in the dataset is imputed using the other variables. These iterations should be run until convergence has been met. Second, after getting the free missing values PM2.5 concentration time series, we get stabilized variance and standard deviation by taking the natural logarithm of each series. Third, the deterministic characteristics containing a linear long-run trend component and yearly seasonality are removed. To accomplish this, model these deterministic components using the following procedure: Let the time series of the PM<sub>2.5</sub> concentration series be donated by  $log(P_d^k)$ ; the super subscript k (k = 1, 2, 3, 4) shows the city series, while d shows the d<sup>th</sup> day data point. Thus, the dynamics of the log daily PM2.5 concentration times series,  $\log(P_d^k)$ , may be described as:

$$log(P_d^k) = \tau_d^k + a_d^k + p_d^k \tag{1}$$

That is, the  $\log(P_d^k)$  in Equation 1 is divided into these components: a long-run linear trend component  $(\tau_d^k)$ , a yearly seasonality component  $(a_d^k)$ , and a residual component  $(p_d^k)$ . The  $(\tau_d^k)$  component is a function of the series (1, 2, 3, ..., d), is estimated by the regression splines method, and dummies capture the annual periodicity:  $a_{d,j}^k = \sum_{j=1}^5 \zeta_j I_{d,j}$ . The variable  $I_{d,j}$  is

assigned a value of 1 when h refers to the i<sup>th</sup> year and 0 otherwise. The regression coefficients ( $\zeta_i$ ) associated with these components are determined using the ordinary least square method. It is worth mentioning that many authors in the literature capture the long-run trend and yearly in a time series using regression splines (Shah et al., 2020; Iftikhar et al., 2023c; Shah et al., 2022; Zhu, 2023; Xu et al., 2022). On the other hand, once the estimated deterministic component (long-run trend and annual periodicity) is obtained, the residual or stochastic component can be derived by using Equation 2:

$$p_d^k = \log(P_d^k) - \left(\hat{\tau}_d^k + \hat{a}_d^k\right) \tag{2}$$

Thus, once the air pollutant (PM<sub>2.5</sub>) concentration time series is preprocessed (to address the issue of missing values and its imputation, stabilize the variance and standard deviation, and remove the deterministic properties), the next step is to model the remaining residual  $p_d^k$  series; the current work considers six single-time series models and three proposed ensemble models. Hence, all forecasting models are described in the coming subsection.

## 2.2 Forecasting models

This section briefly overviews the forecasting models and their proposed ensemble models: the autoregressive, the simple exponential smoothing, the autoregressive moving average, the Theta, the nonparametric autoregressive, and the neural network autoregressive models.

#### 2.2.1 The auto-regressive model

A linear autoregressive (AR) model is used to understand the short-term dynamics of  $p_d$  by using a linear combination of p past observations. The model can be expressed as:

$$p_d = \mathbf{I} + \beta_1 p_1 + \beta_2 p_2 + \dots + \beta_p p_d + \epsilon_d \tag{3}$$

In Equation 3,  $p_i(i = 1, 2, ..., d)$  are observed and past values of PM<sub>2.5</sub>,  $\beta$  AR parameters, and  $\epsilon_m$  is the white noise process. In this study, we estimated the parameters using maximum likelihood estimation. After analyzing the series's auto-correlation function (ACF) and partial auto-correlation function (PACF), we concluded that lags 1, 2, 3, and 7 are significant and, therefore, included in the model (Jenkins and Box, 1976; Box et al., 2015).

#### 2.2.2 The exponential smoothing model

The Exponential Smoothing Model (ESM) is a group of forecasting models that apply exponentially decreasing weights to previous observations. It is a time-series forecasting model that uses a weighted average of past observations to predict the future value of a variable. The ES model assumes that a variable's future value depends on its past values, with greater emphasis placed on recent values than on older ones. The ESM model can be expressed as follows:

$$p_{d+1} = \alpha \cdot p_d + (1 - \alpha) \cdot p_{d-1} \tag{4}$$

In the given Equation 4,  $p_{d+1}$ ,  $p_d$ , and  $p_{d-1}$  are the actual values of the PM<sub>2.5</sub> concentration time series at times d+1, d, and d-1. At the same time,  $\alpha$  is the smoothing parameter determining the weight assigned to the most recent observation (Brown, 1956; Holt, 2004).

#### 2.2.3 The autoregressive moving average model

The autoregressive moving average (ARMA) models incorporate lagged values from a time series and factor in error terms passed into the model. This study utilized a model representing the residual series  $(p_d)$  as a linear combination of d past observations and a delay error term. The model equation can be expressed as:

$$p_d = u + \beta_1 p_1 + \beta_2 p_2 + \dots + \beta_d p_d + \epsilon_n + \xi_1 \epsilon_1 + \xi_2 \epsilon_2 + \dots + x i_s \epsilon_s,$$
(5)

In Equation 5, where *u* is the intercept,  $\beta_i$  (i = 1, 2, ..., d) and  $\xi_j$ , (j = 1, 2, ..., s) are the AR and MA parameters, respectively, and  $\epsilon_d \sim N(0, \sigma_e^2)$ . After conducting graphical analyses (the ACF and PACF plots), this study found that the first two lags are significant in the MA part, while only lags 1, 2, and 7 are significant in the AR part (Jenkins and Box, 1976; Box et al., 2015).

#### 2.2.4 The neural network autoregressive model

The Neural Network Autoregressive (NNA) model is a machine learning approach that uses historical observations to predict future values in a time series. It does this by analyzing a mathematical function that considers the previous values, denoted by  $p_{d-1}, p_{d-2}, \ldots, p_{d-n}$ , where n is the time delay parameter. Training involves the backpropagation method and the steepest descent approach to minimize the difference between predicted and actual values. During the forecasting process, the autoregression order is determined. This order indicates the number of preceding values needed to predict the current time series value. The NNA is then trained using a dataset that reflects the autoregression order, and the number of input nodes is determined based on this order. These inputs represent previous lagged observations in univariate time series forecasting. The NNA's output provides predicted values. However, selecting the number of hidden nodes often involves trial and error and lacks a theoretical basis. Careful consideration is necessary to prevent overfitting when choosing the number of iterations (Taskaya-Temizel and Casey, 2005; Alshanbari et al., 2023). In this study, an NNA design of (4, 2) is utilized, expressed as  $p_d = f(p_{d-1})$ , where  $p_d = (p_{d-1}, p_{d-2}, p_{d-3}, p_{d-4})$ represents past values of the time series of the cleaned daily  $PM_{2.5}$  concentration time series  $(p_d)$ , and f denotes a neural network with four hidden nodes in a single layer.

#### 2.2.5 The nonparametric autoregressive model

The nonparametric autoregressive model (NPAR) presents an alternative to the conventional parametric AR model, departing from the latter's reliance on specific mathematical equations to elucidate the relationship between past and future values. In contrast, NPAR models employ flexible and adaptive techniques, such as kernel regression or spline functions, to capture dynamic patterns in the data without explicit parameter estimation. These models are distinguished by their flexibility, absence of predefined parameters, emphasis on local relationships, and reliance on data-driven structures to address intricate and nonlinear dependencies within time series data. This model's association between  $p_d$  and its previous terms lacks a specific parametric form, allowing for potential non-linearities. This relationship is expressed as:

$$p_{d} = u_{1}(p_{d-1}) + u_{2}(p_{d-2}) + \dots + u_{n}(p_{d-n}) + \varepsilon_{d}$$
(6)

here in Equation 6,  $u_j$  (j = 1, 2, ..., n) denotes smoothing functions describing the association between  $p_d$  and its previous values. In this study, cubic regression splines represent the functions  $u_i$ , and lags 1, 2, 3, and 7 are employed for NPAR modeling (Álvarez-Díaz, 2020; Iftikhar et al., 2023d).

#### 2.2.6 The theta model

The Theta Model is a forecasting method that predicts future values based on the average change in the time series data. It involves calculating the average change between consecutive time points and extrapolating it into the future. The equation for the Theta Model is given by in Equation 7:

$$p_{d+1} = \frac{1}{m} \left( p_d + p_{d-1} + \dots + p_{d-m+1} \right) \tag{7}$$

#### 2.2.7 The proposed ensemble models

At its core, an ensemble technique integrates outcomes from various models, each meticulously calibrated before unity. This approach capitalizes on the inherent strengths of individual models while compensating for their inherent limitations. Within the scope of this study, ensemble techniques are initially employed to compute weights for the results derived from individual models (Iftikhar et al., 2024a; Gonzales et al., 2024). Consequently, the proposed ensemble encompasses three distinct weighting strategies: a) equitable distribution of weight among all single models, denoted as ESME; b) weight assignment based on training average accuracy errors (1), designated as ESMT; and c) weight assignment based on validation mean accuracy measures, denoted as ESMV. The model allocates greater weight to the ensemble model for training and validation datasets with lower mean accuracy errors, while models exhibiting higher mean accuracy errors contribute comparatively less weight to the ensemble. Notably, the model weights assume small positive values, and their accumulation equates to one, signifying the percentage of reliance or anticipated performance from each model.

Thus, after estimating the linear trend component and annual periodicity using the multiple regression model discussed above, the next step is forecasting the remaining part  $(p_d^k)$  using six single and three proposed ensemble models as discussed above. Thus, this work can obtain the daily PM<sub>2.5</sub> concentration for the next day forecast as follows by Equation 8:

$$\hat{P}_d^k = \exp\left(\hat{\tau}_d^k + \hat{a}_d^k + \hat{p}_d^k\right) \tag{8}$$

## 2.3 Evaluation criteria

This study examines two evaluation criteria for the proposed time series ensemble forecasting technique: accuracy average errors and an equal forecast accuracy test.

#### 2.3.1 Accuracy average errors

Primarily, Table 1 presents the accuracy average errors, outlining the formulas for computing each metric. The metrics encompass the mean absolute error (MAE), an indicator of errors within pair samples reflecting the same phenomena. The

TABLE 1 Mea	evaluation	errors.
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S.No	Error	Formula
1	MAE	$\frac{1}{D}\sum_{d=1}^{D} P_D - \hat{P}_D $
2	MASE	$\frac{1}{D} \left[ \frac{ P_D - \hat{P}_D }{1D - 1 \sum_{d2}^{D}  P_D - P_{D-1} } \right]$
3	MAPE	$\frac{1}{D} \sum_{d=1}^{D} \left  \frac{p_D - \hat{p}_D}{p_D} \right $
4	RMSE	$\left[\sum_{d=1}^{D} \left \frac{(D_d - \hat{P}_d)^2}{D}\right]\right]^{0.5}$
5	RMSLE	$\left[\frac{1}{D}\sum_{d=1}^{D} \left[\log(P_d+1) - \log(\hat{P}_d+1)\right]^2\right]^{0.5}$
6	RRSE	$\left[\sum_{d=1}^{D} \frac{(P_d - \hat{P}_d)^2}{\sum_{d=1}^{D} (P_d - \bar{P}_d)^2}\right]^{0.5}$

mean absolute percent error (MAPE) is a metric used to assess how accurate a forecasting system is in making predictions. The mean scaled absolute error (MASE), it is calculated by dividing the mean absolute error of the prediction values by the mean absolute error of the one-step naive forecast made in the sample. The root mean squared error (RMSE) calculates the average disparity between the values a statistical model predicts and the observed values. The root relative squared error (RRSE) root of the squared prediction error in comparison to a simple model that predicts the mean. After applying the log to both, the root mean log squared error (RMSLE) is computed by considering the differences between the actual and anticipated values, Iftikhar et al. (2024b).

The table presents the actual  $(P_d)$  and forecasted  $(\hat{P}_d)$  value of PM<sub>2</sub>.5. Consequently, diminishing values for MAE, MASE, MAPE, RMSE, RRSE, and RMSLE generally signify heightened predictive accuracy of the model.

#### 2.3.2 Equal forecast accuracy test

Second, a statistically equal forecast test, the Diebold–Marino (DM) test (Diebold, 2015), is performed to evaluate the forecasting ensemble time series proposed approach. In the literature, It is used to evaluate time series forecasting models, determining whether the forecast errors from one model are statistically different from another model's forecast errors (Iftikhar et al., 2023a; Shah et al., 2019; Iftikhar et al., 2023b). To perform the DM test, the forecast errors of each model are calculated using a loss function. Then, a statistical value is computed by comparing the errors of each model. The test statistic is based on the difference between the mean squared errors of the two models. Suppose the test statistic is above a certain threshold and the *p*-value is below a significance level ( $\alpha = 0.05$ ). In that case, the forecast from one model are significantly better than the other model. For instance, calculate the forecast errors for both models. Forecast errors ( $e_d = P_d - \hat{P}_d$ ) are



the differences between the observed values  $(P_d)$  and the forecasted values  $(\hat{P}_d)$ . Compute the mean difference  $(\bar{w})$  of the forecast errors:  $\bar{w} = \frac{1}{D}\sum_{d=1}^{D} (e_{1d} - e_{2d})$ . Where:  $e_{1d}$  and  $e_{2d}$  are the forecast errors from Model 1 and Model 2 at time d, respectively, and D is the number of observations. Next, calculate the variance of the differences, such as  $\sigma_d^2 = \frac{1}{D}\sum_{d=1}^{D} (e_{1d} - e_{2d} - \bar{w})^2$ . Thus, the Diebold-Mariano test statistic DM  $= \frac{\bar{w}}{\sqrt{\sigma_d^2}}$ . Finally, the Null and alternative hypothesized generally state as  $H_0$ : There is no difference in forecast accuracy between the two models ( $H_0: \bar{w} = 0$ ) Vs.  $H_A$ : The two models differ in forecast accuracy ( $H_A: \bar{w} \neq 0$ ). Hence, the null hypothesis implies that there is not a statistically significant difference in forecast accuracy between the models. In contrast, the alternative hypothesis suggests a significant difference in forecast accuracy between the two models.

To complete this section, the main steps, including the introduced time series ensemble forecasting approach in bullet form, are listed below, and the flowchart is presented in Figure 1.

• In the first step, we divide the clean PM<sub>2.5</sub> time series data into three parts: training (in-sample), validation (evaluation), and

testing (out-of-sample) datasets. Let  $P_d$ ;  $p = 1, 2, \cdot, D$  (1826) is the PM<sub>2.5</sub> time series. The training (60%, in-sample) dataset is  $P_m$ ;  $m = 1, 2, \cdot, M$  (1096), the validation (20%, evaluation) dataset is  $P_l$ ;  $l = 1, 2, \cdot, L$  (365), and the testing (20%, out-ofsample) dataset is  $P_t$ ;  $t = 1, 2, \cdot, T$  (365) where D (D = M + L + T) is the total data points.

- In the second step, model the train data using single models, i.e., the AR, the ARMA, the ESM, the NPAR, the NNA, and the Theta model.
- In the third step, calculate the one-day-ahead PM<sub>2.5</sub> forecast using the expanding window technique. The forecast values, *P*<sup>j</sup><sub>D−(M+L+T)</sub> for *j* = 1, 2, ⋅, 6, are obtained by the models listed in step 2.
- In the fourth step, the output of a basic ensemble method is mathematically described by Equation 9.

$$\hat{P}_{D-(M+L+T)}^{j} = \sum_{j=1}^{6} W_{i} \hat{P}_{D-(M+L+T)}^{j}$$
(9)

Where  $W_i$ , are obtained by three weighting strategies: a) equal weight to all single models and denoted by (ESME); b) weight assigned based on training mean accuracy measures (MAPE, MASE, MAE, RMSE, RMSLE, and RRSE) and denoted by (ESMT); c) weight assigned based on validation mean accuracy measures and denoted by (ESMV). The lower accuracy mean errors model assigns more weight to the ensemble model in training and validation data sets. In contrast, the model with the model with the highest accuracy has fewer errors than the ensemble model. However, the model weights are small positive values, and the sum of all weights equals one, indicating the percentage of trust or expected performance from each model. Thus, obtain the day-ahead forecast values using Equation 9 for the ESME, ESMT, and ESMV models.

• In the fifth step, evaluate the model based on average accuracy errors, an equal forecast statistical test, and a graphical assessment (see details in 2.3).

## 3 Case study results

In order to obtain short-term PM25 concentration day-ahead forecasts, this study uses the proposed time series ensemble approach to the PM2.5 time series data from major cities in Pakistan, including Karachi, Lahore, Peshawar, and Islamabad. The data in this study was collected primarily from air quality data from sensors located at United States embassies across Pakistan (Pakistan, 2021). The datasets for all four cities (Karachi, Lahore, Peshawar, and Islamabad) were recorded daily for 5 years, from 1 June 2019 to 31 May 2023. The considered datasets are described in Table 2, and the location of each city on the Pakistan map has been shown in Figure 2. However, the PM<sub>2.5</sub> concentration time series generally comprises missing values, high variance, nonnormal, and non-stationary. Before modeling and forecasting, these irregularities must be addressed. To tackle these issues, this work first treated the missing values. Multiple imputations imputed the missing data that were considered using the fully conditionally specified. The imputation was done separately for each series

Data period	City	Total	Observed	Missing	Imputed (%)
2019-2023	Islamabad	1,461	1,430	31	2.12
2019-2023	Lahore	1,461	1,418	43	2.94
2019-2023	Karachi	1,461	1,426	35	2.40
2019-2023	Peshawar	1,461	1,433	28	1.92

TABLE 2 Details about the considered original, missing, and imputed datasets are provided in this work.



(Lahore, Karachi, Peshawar, and Islamabad). The percentage of missing data was between 1.90% and 3.00%, shown in Table 2. However, after getting the imputed  $PM_{2.5}$  concentration time series (free of missing data), Figure 3A depicts a graphical representation of all four cities' imputed daily time series. This figure confirms a long-run linear trend component and an annual seasonality in all four megacities' time series data.

## 3.1 Data description

On the other hand, Table 3 represents a comprehensive overview of the statistical properties (with and without log descriptive statistics) for  $PM_{2.5}$  concentrations of four cities such as Lahore, Peshawar, Karachi, and Islamabad. As a result, these statistics provide valuable insights into the central tendency, spread, symmetry, and stationarity of the data associated with each city. For instance, as seen in this table, the variance and standard deviation are stabilized by taking the logarithm of each city's time series. Conversely, the measures of central tendency (mean, median, and

mode) indicate that the data is non-normal because the mean, median, and mode are unequal. However, the log series in each case shows the same central tendency, indicating that the series is normal by taking the log to the original series in each case. For example, the mean, median, and model for Islamabad city are approximately the same, taking the log of the PM2.5 concentration series. The same experience is experienced in other cities (Lahore, Karachi, and Peshawar). Next, the Augmented Dickey-Fuller (ADF) test is performed to check the nonstationarity issues. The results (the ADF statistic values), listed in Table 3, suggest that both the log-filtered imputed daily PM<sub>2.5</sub> time series and the log-imputed daily PM2.5 time series have a negative statistic value, which indicates that the series is stationary. In addition, the graphical look of all stationary series is plotted in Figure 3B. It can be seen that there is no evidence of nonstationary use in all four megacity time series cases. Once the database addresses all the essential treatments (missing values, variance and standard deviation stabilization, normality, and stationary issues), we proceed further for modeling and forecasting purposes. The dataset was divided into training, validation, and



testing datasets. For the daily PM2.5 concentration forecast, the training dataset (fitting model) was 3 years (60%) from 1 June 2019 to 31 May 2021, while the validation (validation model, 20%) and testing (testing model, 20%) datasets were one complete year from 1 June 2021 to 31 May 2022 and 1 June 2022 to 31 May 2023, respectively.

FIGURE 3

Statistic	Islamabad	Lahore	Karachi	Peshawar	log (Islamabad)	log (Lahore)	log (Karachi)	log (Peshawar)
Minimum	10.00	5.00	9.00	16.00	2.30	1.61	2.20	2.77
Maximum	270.00	503.00	277.00	557.00	5.60	6.22	5.62	6.32
25%	84.00	128.00	77.00	112.00	4.43	4.85	4.34	4.72
50%	106.00	162.00	97.00	142.00	4.66	5.09	4.57	4.96
75%	139.00	218.00	143.00	168.00	4.93	5.38	4.96	5.12
Mean	112.34	183.15	109.97	146.01	4.65	5.10	4.62	4.92
Variance	1,576.95	7257.72	1795.17	2662.09	0.15	0.25	0.16	0.13
Standard Deviation	39.71	85.19	42.37 51.	51.60	0.39	0.50	0.40	0.36
Skewness	0.43	1.12	0.67	1.44	-1.03	-1.43	-0.66	-0.92
Kurtosis	2.94	4.18	2.76	8.60	6.23	11.44	6.43	7.95
ADF Statistic	-4.05	-4.24	-3.66	-4.68	-4.54	-5.02	-4.34	-5.37
D_ADF Statistic	-16.97	-16.12	-16.82	-17.38	-17.42	-15.85	-16.57	-16.20

#### TABLE 3 Descriptive statistics.

## 3.2 PM<sub>2.5</sub> forecasting outcomes

The given steps must be followed to obtain the forecast for PM2.5 concentration one step ahead of a day using the proposed time series ensemble forecasting technique presented in Section 2. First, the time series of PM2.5 is preprocessed by missing values and their imputation, variance and standard deviation stabilization, deterministic properties (trend and seasonality), and stationary concerns are addressed. Then, six single time series and three ensemble models anticipate the cleaned PM2.5 concentration time series. Therefore, the forecast of a day ahead was obtained using the expanding window technique for 365, and the models were estimated accordingly. Finally, the PM2.5 concentration forecasts were achieved through Equation 9. The performance measures, including MAE, MASE, MAPE, RMSE, RRSE, and RMSLE, are then used for the evaluation and comparative performance of the models. Hence, this work uses six single time series models, including the autoregressive model, the exponential smoothing model, the autoregressive moving averages, the nonlinear autoregressive, the neural network autoregressive, and the theta model, and three proposed ensemble models (the ESME, the ESMT, and the ESMV). Thus, the proposed time series ensemble forecasting approach compares nine total models within the two contexts, such as comparing single model performance, the proposed ensemble models, and single verse ensemble models.

Hence, for all nine models for the four monitoring megacities, including Lahore, Islamabad, Karachi, and Peshawar, one-day-ahead out-of-sample forecast outcomes (MAE, MASE, MAPE, RMSE, RRSE, and RMSLE) are listed in Table 4. Table 4 shows that the ESMV produced the best forecasting results compared to all nine forecasting models within the proposed time series ensemble forecasting approach in all four monitoring megacities. For instance, the average accuracy errors for these magacities are the following: Islamabad (MAPE = 0.1739, MAE = 15.2718, MASE = 0.9237, RMSE = 20.3203, RRSE = 0.4830, and RMLSE = 0.2354); Lahore

(MAPE = 0.2167, MAE = 34.1786, MASE = 0.9207, RMSE = 48.3090, RRSE = 0.5837, and RMLSE = 0.2701); Karachi (MAPE = 0.1679, MAE = 16.0982, MASE = 0.9122, RMSE = 22.9913, RRSE = 0.5464, and RMLSE = 0.2215); and Peshawar (MAPE = 0.1973, MAE = 24.1188, MASE = 0.8858, RMSE = 35.0552, RRSE = 0.5998, and RMLSE = 0.2594). However, the ESMT model shows the second-best forecasting results among all nine forecasting models in all four monitoring megacities, while the third-best forecasting accuracy average error results are given in the following manner: Islamabad (the Theta model; MAPE = 0.1835, MAE = 16.3457, MASE = 0.9887, RMSE = 21.2335, RRSE = 0.5047, and RMLSE = 0.2370; Lahore (the Theta model; MAPE = 0.2179, MAE = 35.0539, MASE = 0.9442, RMSE = 49.9617, RRSE = 0.6037, and RMLSE = 0.2723); Karachi (the ARMA model; MAPE = 0.1702, MAE = 16.3909, MASE = 0.9287, RMSE = 23.3728, RRSE = 0.5555, RMSLE = 0.2226); and Peshawar (the NPAR model; MAPE = 0.2010, MAE = 25.0597, MASE = 0.9204, RMSE = 36.1912, RRSE = 0.6037, and RMLSE = 0.2723); Karachi (the ARMA model; MAPE = 0.1702, MAE = 16.3909, MASE = 0.9287, RMSE = 23.3728, RRSE = 0.5555, RMSLE = 0.2226); and Peshawar (the NPAR model; MAPE = 0.2010, MAE = 25.0597, MASE = 0.9204, RMSE = 36.1912, RRSE = 0.6192, RMSLE = 0.2610). Therefore, it is seen that within all nine forecasting models, the proposed ensemble models (the ESMV and the ESMT models) generally perform better than single models; however, within the single models, different cities have different single best models, as mentioned previously. Note that the best model is an ESMV or equivalent for all four mountaineering megacities. Also, using the proposed ensemble learning leads to marked error reduction (see Table 4). The proposed ensemble learning approach, thus, proves to be particularly effective in forecasting short-term  $\mathrm{PM}_{2.5}$  concentration.Once the best models are achieved by average accuracy errors, they are processed to confirm their superiority using a statistical test; for this purpose, this work performs the Diebold and Mariano test (DM). This test is

TABLE 4 The average accuracy errors for all six single models and three proposed ensemble models.

Islamabad											
Model	MAPE	MAE	MASE	RMSE	RRSE	RMLSE					
AR	0.1904	17.2904	1.0458	22.5284	0.5355	0.2454					
ARIMA	0.1864	16.7744	1.0146	21.7228	0.5164	0.2399					
ESM	0.1893	16.9394	1.0246	22.8407	0.5429	0.2633					
NNA	0.2188	19.2108	1.1620	25.1802	0.5986	0.2794					
NPAR	0.1922	16.8240	1.0176	21.6783	0.5153	0.2462					
Theta	0.1835	16.3457	0.9887	21.2335	0.5047	0.2370					
ESME	0.1934	17.2308	1.0422	22.5306	0.5356	0.2519					
ESMT	0.1802	15.4959	0.9373	20.5671	0.4889	0.2441					
ESMV	0.1739	15.2718	0.9237	20.3203	0.4830	0.2354					
LAHORE											
AR	0.2229	36.8529	0.9927	52.3530	0.6326	0.2887					
ARIMA	0.2231	36.8117	0.9916	51.9208	0.6273	0.2785					
ESM	0.2253	37.3232	1.0054	53.5939	0.6475	0.2889					
NNA	0.2461	40.2607	1.0845	58.0993	0.7020	0.3098					
NPAR	0.2185	36.0432	0.9709	51.1469	0.6180	0.2768					
Theta	0.2179	35.0539	0.9442	49.9617	0.6037	0.2723					
ESME	0.2256	37.0576	0.9982	52.8459	0.6385	0.2858					
ESMT	0.2174	34.4391	0.9277	48.6824	0.5882	0.2706					
ESMV	0.2167	34.1786	0.9207	48.3090	0.5837	0.2701					
			KARACHI								
AR	0.1742	16.8161	0.9528	24.1719	0.5745	0.2294					
ARIMA	0.1702	16.3909	0.9287	23.3728	0.5555	0.2226					
ESM	0.1763	17.0864	0.9682	24.6113	0.5849	0.2325					
NNA	0.1782	16.9910	0.9628	24.0124	0.5707	0.2292					
NPAR	0.1758	16.6460	0.9432	23.7852	0.5653	0.2270					
Theta	0.1745	16.4752	0.9335	23.1691	0.5506	0.2219					
ESME	0.1749	16.7343	0.9482	23.8538	0.5669	0.2271					
ESMT	0.1732	16.2855	0.9228	23.2569	0.5527	0.2229					
ESMV	0.1679	16.0982	0.9122	22.9913	0.5464	0.2215					
		F	PESHAWAF	2							
AR	0.2043	26.3133	0.9664	38.2363	0.6542	0.2728					
ARIMA	0.2064	26.4649	0.9720	37.4996	0.6416	0.2653					
ESM	0.2102	27.0384	0.9930	38.8519	0.6648	0.2797					
NNA	0.2080	25.9315	0.9524	38.0994	0.6519	0.2682					
NPAR	0.2010	25.0597	0.9204	36.1912	0.6192	0.2610					
Theta	0.2031	25.3092	0.9295	37.1880	0.6363	0.2629					
ESME	0.2055	26.0195	0.9556	37.6777	0.6447	0.2683					
ESMT	0.1988	24.8234	0.9117	35.8784	0.6139	0.3949					
ESMV	0.1973	24.1188	0.8858	35.0552	0.5998	0.2594					

used to check whether two different models performed in the same way or vice versa, and the following hypotheses are tested: the null hypothesis, H<sub>0</sub>: There is equal accuracy between the models on the rows and columns; the alternative, H<sub>A</sub>: Compared to the models on the rows, the models on the columns are more accurate. In this way, the hypothesis's testing is statistically evaluated with the *p*-value. The models assessed by this test can be interpreted as indicating that the higher the *p*-value, the better the performance of the specific model. The results (p-values) are demonstrated in Table 5, and the evaluation of these results is based on the row and column in each case. For example, for the Islamabad city in Table 5, it can be noticed that the proposed ensemble model ESMV outperforms the existing models with a value of 0.9120; additionally, for the Lahore station in Table 5, it can be observed that the proposed ensemble model ESMV outputs a significant *p*-value of 0.900, which shows that the proposed ensemble model is more efficient than others. Furthermore, for the Karachi station in Table 5, it is noticed that the proposed ensemble model shows a significant value of 0.908. In addition to this, for the Peshawar station in Table 5, it can be noticed that the proposed ensemble model results in a p-value of 0.908, which is more significant than other models. Hence, again, it is confirmed by the statistical test that the proposed ensemble model performed better in the prediction of PM2.5 than the existing models for all four megacities.

On the other hand, after the evaluation of the proposed time series ensemble modeling and forecasting technique by the average mean errors and the DM test, another check can be made to evaluate the accuracy of the selected best ensemble models by the graphical representation of the observed data and the predicted data. To do this, each city's scatter plot (correlation) is drawn, and the correlation coefficient is calculated. Figures 4A-D shows the graph for each megacity. In Figure 5A for Islamabad city, it is noticed that the correlation coefficient value between the forecasted and actual data set is 0.97, indicating a strong and positive correlation. Moreover, from Figure 4B for Lahore city, the coefficient value between forecasted and actual data is 0.86, which shows a strong positive correlation between forecasted and actual data. Figure 4C for Karachi city and Figure 4D for Peshawar city, the coefficient values are 0.85 and 0.94, which shows a strong positive correlation between forecasted and actual data. In addition, the diagnostic checking (final residuals) plays an essential role in model selection, and this is tracked by the auto-correlation (ACF) plot and the partial auto-correlation plot (PACF), also known as the correlogram plot. As stated earlier, the proposed ensemble model is significant and efficient in forecasting the PM2.5 concentration, so the proposed ensemble model ESMV residuals are plotted using correlograms (ACF and PACF plots). In Figure 5, the Figure 5A, C, E, G and Figure 5B, D, F, H plots of four megacities, namely, Islamabad, Lahore, Karachi, and Peshawar, are demonstrated, and the 95% of the confidence interval is calculated, which is shown by the dashed (-) lines for the upcoming lags. This Figure 5 shows that no spike is out of the 95% of the C.I. for all four cities, indicating that the residuals are white noise and the selected model is best for the further statistical perspective, i.e., prediction and forecast.Hence, to sum up this section, based on the evaluation criteria (average mean errors, the statistical test, and the graphical assessment), the proposed time series ensemble forecasting approach is best for efficient and accurate short-term forecasts for PM<sub>2.5</sub> concentration forecasting. In addition, within the proposed time series ensemble learning approach, the proposed ESMV model

Islamabad												
Model	AR	ARIMA	ESM	NNA	NPAR	Theta	ESME	ESMT	ESMV			
AR	0.000	0.102	0.540	0.903	0.108	0.097	0.095	0.091	0.091			
ARIMA	0.898	0.000	0.845	0.902	0.465	0.092	0.087	0.088	0.088			
ESM	0.460	0.155	0.000	0.910	0.163	0.125	0.127	0.103	0.102			
NNA	0.098	0.098	0.090	0.000	0.099	0.097	0.097	0.094	0.094			
NPAR	0.892	0.535	0.837	0.901	0.000	0.088	0.089	0.087	0.087			
Theta	0.903	0.908	0.875	0.903	0.912	0.000	0.888	0.087	0.087			
ESME	0.905	0.913	0.873	0.903	0.911	0.112	0.000	0.088	0.089			
ESMT	0.909	0.912	0.897	0.906	0.913	0.913	0.912	0.000	0.091			
ESMV	0.909	0.912	0.898	0.906	0.913	0.913	0.911	0.909	0.000			
Lahore												
Model	AR	ARIMA	ESM	NNA	NPAR	Theta	ESME	ESMT	ESMV			
AR	0.000	0.165	0.873	0.891	0.104	0.099	0.099	0.104	0.104			
ARIMA	0.835	0.000	0.865	0.889	0.091	0.094	0.089	0.100	0.100			
ESM	0.127	0.135	0.000	0.895	0.114	0.107	0.110	0.109	0.108			
NNA	0.109	0.111	0.105	0.000	0.108	0.106	0.107	0.107	0.107			
NPAR	0.896	0.909	0.886	0.892	0.000	0.096	0.114	0.105	0.104			
Theta	0.901	0.906	0.893	0.894	0.904	0.000	0.900	0.117	0.113			
ESME	0.901	0.911	0.890	0.893	0.886	0.100	0.000	0.108	0.107			
ESMT	0.896	0.900	0.891	0.893	0.895	0.883	0.892	0.000	0.102			
ESMV	0.896	0.900	0.892	0.893	0.896	0.887	0.893	0.898	0.000			
				Kai	rachi							
Model	AR	ARIMA	ESM	NNA	NPAR	Theta	ESME	ESMT	ESMV			
AR	0.000	0.113	0.893	0.437	0.121	0.131	0.098	0.109	0.107			
ARIMA	0.887	0.000	0.889	0.908	0.893	0.274	0.262	0.093	0.099			
ESM	0.107	0.111	0.000	0.155	0.113	0.122	0.101	0.109	0.107			
NNA	0.563	0.092	0.845	0.000	0.087	0.107	0.087	0.093	0.094			
NPAR	0.879	0.107	0.887	0.913	0.000	0.138	0.089	0.103	0.102			
Theta	0.869	0.726	0.878	0.893	0.862	0.000	0.565	0.400	0.092			
ESME	0.902	0.738	0.899	0.913	0.911	0.435	0.000	0.280	0.136			
ESMT	0.891	0.907	0.891	0.908	0.897	0.600	0.720	0.000	0.102			
ESMV	0.893	0.901	0.893	0.906	0.898	0.908	0.864	0.898	0.000			
				Pesl	nawar							
Model	AR	ARIMA	ESM	NNA	NPAR	Theta	ESME	ESMT	ESMV			
AR	0.000	0.223	0.912	0.100	0.108	0.093	0.112	0.107	0.103			
ARIMA	0.777	0.000	0.878	0.612	0.090	0.111	0.087	0.091	0.092			
ESM	0.089	0.122	0.000	0.087	0.100	0.091	0.100	0.100	0.099			

#### TABLE 5 The DM test outcomes for all six single models and three proposed ensemble models.

(Continued on following page)

Peshawar												
Model	AR	ARIMA	ESM	NNA	NPAR	NPAR Theta		ESMT	ESMV			
NNA	0.900	0.388	0.913	0.000	0.120	0.104	0.134	0.117	0.109			
NPAR	0.892	0.910	0.900	0.880	0.000	0.857	0.900	0.101	0.097			
Theta	0.907	0.889	0.909	0.896	0.143	0.000	0.305	0.129	0.112			
ESME	0.888	0.913	0.900	0.866	0.100	0.695	0.000	0.100	0.098			
ESMT	0.893	0.909	0.900	0.883	0.899	0.871	0.900	0.000	0.096			
ESMV	0.897	0.908	0.901	0.891	0.903	0.888	0.902	0.904	0.000			

TABLE 5 (Continued) The DM test outcomes for all six single models and three proposed ensemble models.



produces more precise forecasts when compared with the alternative ensemble models and single time series models.

 $\mathrm{PM}_{2.5}$  forecasting results and directions for the policymaker and health sector precautions.

## 4 Discussion

This section elaborates an overview of comparing the proposed best model of this work *versus* the literature that found the best forecasting models. On the other hand, it also explains the future

## 4.1 Comparatively study resutls

In this subsection, we compared the results of our best ensemble model with those reported in the literature models. Our model showed high comparability with the other methods. Our best



#### FIGURE 5

The autocorrelation function and partial autocorrelation plots for the best models among all nine considered models in each megacity case: (A, B) Islamabad, (C, D) Lahore, (E, F) Karachi, (G, H) Peshawar.

(ESMV) model produced the most negligible mean errors and the highest correlation coefficient (MAPE = 0.1679, MAE = 16.0982, MASE = 0.9122, RMSE = 22.9913, RRSE = 0.5464, and RMLSE =

0.2215) compared to the best models reported in the literature. For example, the best autoregressive distributed lag model (the ARDL model) proposed in Qayyum et al. (2021) was applied to the dataset

		-		-	-								
Islamabad			Karachi				Lahore			Peshawar			
Date	Actual	Forecasted	PFE	Actual	Forecasted	PFE	Actual	Forecasted	PFE	Actual	Forecasted	PFE	
6/1/2023	49.00	48.12	1.80	55.00	54.60	0.73	93.00	92.03	1.04	73.00	73.02	0.03	
6/2/2023	76.00	76.50	0.66	63.00	64.01	1.60	139.00	138.01	0.71	96.00	95.09	0.95	
6/3/2023	79.00	79.32	0.41	70.00	70.43	0.61	153.00	153.90	0.59	128.00	127.91	0.07	
6/4/2023	90.00	88.12	2.09	80.00	81.01	1.26	126.00	125.01	0.79	113.00	112.01	0.88	
6/5/2023	83.00	82.10	1.08	62.00	62.98	1.58	123.00	124.01	0.82	100.00	99.09	0.91	
6/6/2023	83.00	82.30	0.84	60.00	59.02	1.63	88.00	89.01	1.15	121.00	120.76	0.20	
6/7/2023	86.00	84.50	1.74	64.00	64.98	1.53	125.00	124.21	0.63	129.00	129.09	0.07	
6/8/2023	113.00	113.54	0.48	65.00	65.02	0.03	236.00	237.50	0.64	124.00	125.01	0.81	
6/9/2023	125.00	123.12	1.50	60.00	59.02	1.63	174.00	174.50	0.29	153.00	154.05	0.69	
6/10/2023	107.00	107.54	0.50	60.00	60.09	0.15	145.00	144.30	0.48	148.00	148.04	0.03	
6/11/2023	80.00	81.00	1.25	50.00	51.23	2.46	118.00	118.09	0.08	102.00	102.98	0.96	
6/12/2023	100.00	99.98	0.02	72.00	72.90	1.25	147.00	146.32	0.46	132.00	132.12	0.09	
6/13/2023	104.00	103.20	0.77	75.00	74.08	1.23	133.00	132.05	0.71	116.00	116.12	0.10	
6/14/2023	91.00	90.12	0.97	73.00	72.58	0.58	116.00	116.43	0.37	134.00	134.76	0.57	
6/15/2023	67.00	65.98	1.52	76.00	75.55	0.59	89.00	89.02	0.02	83.00	84.09	1.31	

TABLE 6 Forecasted values exercise for all megacities for the next 15 days using the best model in each case.

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used in our study and showed accuracy measures (MAPE = 0.1835, MAE = 21.3457, MASE = 0.9887, RMSE = 21.2335, RRSE = 0.5047, and RMLSE = 0.2370) that were significantly greater than those of our best (ESMV) model. The best model proposed in another study (see Bhatti et al., 2021) - the seasonal autoregressive moving average factor analysis approach - was also applied to our dataset and obtained average mean errors (MAPE = 0.1823, MAE = 20.1038, MASE = 0.9483, RMSE = 36.1853, RRSE = 0.7214, and RMLSE = 0.2901) that were higher than those of our best (ESMV) model. Similarly, in reference Waseem et al. (2022), the best proposed LSTM encoder-decoder applied to our dataset obtained performance metrics (MAPE = 0.2010, MAE = 25.0597, MASE = 0.9204, RMSE = 36.1912, RRSE = 0.6192, RMSLE = 0.2610) worse than those obtained with our best combination model (ESMV). In conclusion, our study's best final model (ESMV) showed high efficacy and accuracy compared to the best models reported in the literature.

## 4.2 Future short-term forecasting using the superior model

On the other hand, once the best models were assessed through average accuracy errors (MAPE, MAE, MASE, RMSLE, RRSE, and RMSE), an equal forecast statistical test (the DM test), graphical evaluation (the ACF, PCAF, and correlogram plots), and comparing with the literature best models this work proceeded to future shortterm forecasting with the superior model (the ESMV). In this regard, the current work used the ESMV for the PM2.5 concentration and forecast from June 1 to 15 June 2023 (15 days) for the daily PM2.5 concentration. The forecasted and actual values of the daily PM25 concentration are tabulated in Table 5. As seen from this table, the daily PM<sub>2.5</sub> concentration gradually increased, and the first peak (123.12  $(\mu g/m^3)$ ) was attained on 9 June 2023; however, after this peak, the forecasts were between 65  $(\mu g/m^3)$  and 110  $(\mu g/m^3)$ . In Lahore city's case, the highest value (236.00  $(\mu g/m^3)$ ) of PM<sub>2.5</sub> was observed on 8 June 2023, while the other days also showed higher and worse air quality throughout the 15 days. Conversely, Karachi City has observed moderate PM<sub>2.5</sub> concentration levels between 50  $(\mu g/m^3)$  and 80  $(\mu g/m^3)$  throughout the next 15 days. In the case of Peshawar City, the PM2.5 concentration level was not healthy, and the highest peak was observed on 9 June 2023; however, the other 14 days also showed significant polluted air in the city. As the proposed ensemble model passes all the necessary statistical tests to prove its efficiency over the other existing models that are being compared, the final step is to move towards daily forecasted PM2.5 concentration values versus the original PM2.5 concentration values of the 15 days (June 1 to 15 June 2023). Table 6 presents the forecasted values for the next 15 days for all four megacities using the proposed model. The percentage forecast error (PFE) is calculated, while the PFE can be defined as PFE =  $(\hat{P} - P/P) * 100$ . where P is the actual value and  $\hat{P}$  stands for forecasted values. Table 6 gives PFE for each city for the next 15 days. It is found that, on average, the PFE for Islamabad station is 1.04, which is negligible, or stated differently, that this error lies in a 95% confidence interval. Also, for the Karachi station, the PFE on average is 1.12. Moreover, the PFE on average for Lahore station is 0.58, and lastly, for Peshawar station, the PFE on average is 0.51. These, on average, errors prove that the proposed ensemble model forecasts the  $\mathrm{PM}_{2.5}$  efficiently with the lowest forecast errors.

As per the Air Quality Index by the Environment Protection Agency, US, the following ranges and their health level concerns: 0 - 12 $(\mu g/m^{3}),$ good; 12.1-34.5  $(\mu g/m^3),$ moderate; 34.6-55.4  $(\mu g/m^3),$ unhealthy for sensitive groups; 55.5-150.4  $(\mu g/m^3)$ , unhealthy; 150.5–250.4  $(\mu q/m^3)$ , very unhealthy; 250.5-350.4  $(\mu g/m^{3}),$ and hazardous; 350.5-450.4 ( $\mu q/m^3$ ). In this way, the air quality is classified into different categories for the four megacities of Pakistan based on actual and forecasted values. Islamabad city found that most of the predicted values lie in the fourth class, i.e.,  $\geq$  55.5, which indicates that the air in Islamabad is unhealthy and needs severe precautions for the citizen's health. Moreover, for Karachi, it is found from the forecasted table that the most values lie in the third class, i.e.,  $\leq$ 55.5  $(\mu g/m^3)$ , which highlights that the air of the Karachi district is sensitive to some specific groups of people. In addition to this, for Lahore city, the majority of forecasted values lie in the, i.e.,  $\leq$ 55.5  $(\mu g/m^3)$  unhealthy and, i.e.,  $\leq 150.5 (\mu g/m^3)$  very unhealthy class of air quality, and lastly, for Peshawar city, the majority of predicted values lie in the suffering class of air quality. Therefore, given that the study demonstrated that ensemble-based time series models could reliably simulate and forecast PM2.5 levels, it is suggested that these models be used in real-world scenarios. These models can help decision-making about pollution control and public health by offering insight into future PM<sub>2.5</sub> levels. Policymakers can benefit from precise PM2.5 forecasts when creating efficient pollution management strategies and regulations. To detect trends and patterns and implement timely measures to alleviate pollution and its detrimental impacts on public health, regular monitoring of PM2.5 levels in Pakistan's main cities might be helpful. The study's findings can be utilized to educate the public about the dangers increased PM<sub>2.5</sub> levels pose to their health. Public awareness efforts concerning PM2.5 pollution can help people decrease their exposure by encouraging them to use air purifiers indoors and stay indoors during high pollution. In summary, this study offers a significant understanding of the modeling and forecasting of PM<sub>2.5</sub> levels in Pakistan's main cities, which may guide policy decisions and measures to lower air pollution and safeguard public health.

## 5 Conclusion

This work proposes a novel time series ensemble approach using the daily PM2.5 concentration data from 1 January 2019 to 31 May 2023 from Pakistan's megacities, including Lahore, Karachi, Peshawar, and Islamabad, to forecast short-term PM<sub>2.5</sub> concentrations. First, the proposed ensemble approach preprocesses the PM2.5 time series by missing value, variance stabilization, normality, deterministic features, and stationary concerns. Second, six single forecasting models: four linear (autoregressive, simple exponential smoothing, autoregressive moving average, and theta) and two nonlinear (nonparametric autoregressive and neural network autoregressive) time series models and three of their ensemble models forecast the cleaned PM<sub>2.5</sub> concentration time series. The results of six accuracy metrics, the Diebold and Mariano test, and the correlation plot show that the proposed ensemble approach, ESMV, was accurate and efficient for day-ahead  $PM_{2.5}$  concentration forecasting. For instance, when the performance of the best ensemble model (ESMV) was compared to all the competitor models (six single models and two other proposed ensemble models) in the four monitoring cities, it was discovered that the model performance had mean errors ranging from 3.60% to 25.79%, 0.81%–13.52%, 1.08%–7.06%, and 1.09%–12.11% in Islamabad, Lahore, Karachi, and Peshawar.

In addition, using the best ensemble model in this work, a forecast was made for the next 15 days (1 June to 15 June 2023); the forecast exercise shows that the elevated levels of PM25 in major megacities of Pakistan, including Islamabad, Lahore, Karachi, and Peshawar, are suffering from severe air pollution issues. The capital city of Pakistan, Islamabad, is significantly affected by the problem of air pollution, with exceptionally high PM2.5 levels, and the leading cause of this pollution belongs to multiple sources, including industrial processes, natural sources, and vehicle emissions. Another significant city in Pakistan, Lahore, has frequently experienced considerable trouble with its air quality, notably in the winter season when variables like temperature inversions and crop burning increase pollution levels. Being a major metropolis and an industrial center, Karachi also suffers from air pollution. The reasons behind this air pollution are the city's industrial operations, heavy traffic, and trash burning. Peshawar, a capital city in the province of Khyber Pakhtunkhwa, also has air pollution problems, and the same factors, like automobile emissions, manufacturing, and farming practices, cause air pollution. It was found that the factors that pollute the air and make it unhealthy are similar in every city in Pakistan. This polluted air caused smog and irregular moments like accidents and holidays at educational institutions.

However, the study's main limitation is that it only incorporates  $PM_{2.5}$  concentration data and does not include additional exogenous parameters such as temperature,  $PM_{10}$ , wind speed, ozone concentration, meteorological data, and gas concentrations, which might improve  $PM_{2.5}$  forecasting accuracy. On the other hand, the current study employed only data from Pakistani megacities. It may be used in different countries to assess the utility of the proposed time series ensemble modeling and forecasting approach. Furthermore, while this study only employed univariate time series models, machine learning techniques like deep learning and artificial neural networks might be explored within the proposed forecasting framework.

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## Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

## Author contributions

HI: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing–original draft, Writing–review and editing. MQ: Data curation, Formal Analysis, Investigation, Writing–review and editing. JZ: Funding acquisition, Project administration, Supervision, Writing–review and editing. JL-G: Investigation, Project administration, Resources, Supervision, Writing–review and editing. OA: Investigation, Resources, Supervision, Writing–review and editing.

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## Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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