Analytical Equations based Prediction Approach for PM2.5 using Artificial Neural Network

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Abstract Particulate matter pollution is one of the deadliest types of air pollution worldwide due to its significant impacts on the global environment and human health. Particulate Matter (PM2.5) is one of the important particulate pollutants to measure the Air Quality Index (AQI). The conventional instruments used by the air quality monitoring stations to monitor PM2.5 are costly, bulkier, time-consuming, and power-hungry. Furthermore, due to limited data availability and non-scalability, these stations cannot provide high spatial and temporal resolution in real-time. To overcome the disadvantages of existing methodology this article presents analytical equations based prediction approach for PM2.5 using an Artificial Neural Network (ANN). Since the derived analytical equations for the prediction can be computed using a Wireless Sensor Node (WSN) or low-cost processing tool, it demonstrates the usefulness of the proposed approach. Moreover, the study related to correlation among the PM2.5 and other pollutants is performed to select the appropriate predictors. The large authenticate data set of Central Pollution Control Board (CPCB) online station, India is used for the proposed approach. The RMSE and coefficient of determination ($R^2$) obtained for the proposed prediction approach using eight predictors are 1.7973 $\mu$g/m$^3$ and 0.9986 respectively. While the proposed approach results show RMSE of 7.5372 $\mu$g/m$^3$ and $R^2$ of 0.9708 using three predictors. Therefore, the results demonstrate that the proposed approach is one of the promising approaches for monitoring PM2.5 without power-hungry gas sensors and bulkier analyzers.

Keywords Prediction Model, PM2.5, Correlation, Artificial Neural Network, Air Pollution Monitoring, Machine Learning

1 Introduction

Meteorological parameters such as temperature, humidity, light, air velocity and gaseous pollutants such as Carbon Dioxide (CO$_2$), Carbon Monoxide (CO), Nitrogen Dioxide (NO$_2$), Sulphur Dioxide (SO$_2$), Volatile Organic Compounds (VOCs), Suspended Particulate Matter (SPM), and Ozone (O$_3$) express the environment quality. The main sources of these pollutants are industrial, residential, transportation, trading, agricultural, and natural activities such as combustion of fuels, wood fire, and forest fire, etc. [1][2]. In India, the Central Pollution Control Board (CPCB) is responsible for providing the ambient Air Quality Index (AQI) through the National Air Quality Monitoring Programme (NAMP). The NAMP network consists of approximately 683 monitoring stations deployed across 300 cities/towns in 29 states and 6 union territories of the country. The objectives of NAMP are to determine the status and trends of ambient air quality and check the prescribed upper and lower limits of the air quality and take corrective measures for the AQI [3]. The AQI transforms the air quality data into a number, nomenclature, color,
Outdoor Monitoring

Direct Methods

Analyzer \[10\]
Aethalometer \[12\]
Sampler \[13\]-\[15\]
WSN \[16\]-\[19\]

Indirect Methods

Prediction model based on past data of predictand, meteorological parameters and other pollutants \[21\]-\[45\]
Prediction model based on correlated meteorological parameters and pollutants \[46\]-\[48\]

Proposed Method
(Prediction model based on correlated pollutants, as analytical equations)

Fig. 1 Direct and Indirect Methods of Prediction of Pollutants for Outdoor Monitoring

and a category; Good, Satisfactory, Moderately Polluted, Poor, Very Poor and Severe based on their health impacts. The overall AQI \[5\] is calculated from a minimum three pollutants out of which one should be the Particulate Matter (PM2.5) which can potentially cause serious health problems.

PM2.5 poses a major concern for human health as due to its small size (< 2.5µm) they can directly enter into the lungs \[6\]. PM2.5 comes either from primary sources or from secondary sources. The primary sources can be vehicles, power plants, wood burning, industrial processes, forest or grass fires, and agricultural burning processes. The secondary sources are precursor emissions such as Sulfur dioxide (SO\(_2\)), Oxides, Volatile Organic Compounds (VOCs), and Ammonia (NH\(_3\)) \[6, 7\]. Though different methods and instruments for monitoring PM2.5 exist \[8\], only a few are used for real-time measurement and monitoring. These instruments for PM2.5 often lack portability and exhibit a slower response time \[9\]. Furthermore, the standard procedure to collect samples through samplers and analyzing them offline in specialized laboratories is challenging for real-time monitoring and corrective actions \[10\]-\[11\]. This is because analyzed data is a delayed response of the current data. Hence real-time monitoring of PM2.5 can be useful. In this work, we propose a method to address the issue of the delayed response of data. We propose the PM2.5 prediction model based on analytical equations, which can be ported to a standard Wireless Sensor Node (WSN). We envisage that such a method not only provides benefits for real-time monitoring but also enables an existing WSN to extend its capabilities from monitoring to analyzing.

2 Related Work

The classification of both direct and indirect measurements for outdoor environmental monitoring is shown in Fig. \[1\] In direct methods, dedicated instruments such as analyzers \[10\], aethalometer \[12\], samplers \[13\]-\[15\], and in certain cases Wireless Sensor Nodes (WSNs) \[16\]-\[19\] are used. Aethalometer and analyzers provide the pollutants’ values directly but lack portability and are often expensive. In air pollution monitoring using samplers, offline analysis is done in specialized laboratories. Whereas in wireless sensor nodes, the measurement of pollutants is done using on-board gas sensors and is often a cost-effective solution compared to other monitoring methods \[20\]. An example of such a system deployed in a New York subway is discussed in \[12\].

The indirect measurements \[21\]-\[37\], \[39\]-\[45\] used prediction approach based on the past data of the predictand, pollutants and/or meteorological parameters. These pollutants and meteorological parameters are correlated with the predictand \[38\]-\[46\]. The PM2.5 (predictand) can be forecasted based on the data of pollutants and meteorological parameters which are correlated with PM2.5. The performance comparison of different prediction techniques of greenhouse gas is discussed in \[49\]. In \[21\], a comparison of different topologies of a neural network is presented for a prediction model of PM2.5. A neural network-based prediction model for PM10 using previous days data for PM10, cloud cover, boundary layer height, wind direction and day of the week is discussed in \[22\]. For the prediction of PM2.5 and O\(_3\), the empirical non-linear regression model was designed \[24\] using meteorological parameters and
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past PM2.5 data. In [24] feed-forward neural network is used for prediction of PM2.5 based on past values of PM10, PM2.5 and some observed and forecasted meteorological parameters. In [25, 26], prediction based on ANN using past data of O3 is discussed. A Multilayer Perceptron (MLP) neural network-based prediction model [27] for NO and NO2 pollutants is developed using past data of pollutants. In [28] prediction model show MLP neural network has better performance than Multiple Linear Regression (MLR) model. Results in [29] demonstrates the better performance of ANN compared to MLR for prediction of PM2.5 in the agricultural park. Comparison results of MLR and ANN in [30] for prediction of PM2.5 represents the better performance of ANN. Feed Forward Neural Network (FFNN) with Rolling Mechanism (RM) and Accumulated Generating Operation (AGO) of Gray model (RM-GM-FFNN) was developed [31] for prediction of PM2.5 and PM10 using past data of PM2.5 and PM10 in addition to meteorological data. Prediction of PM2.5 based on the Back Propagation (BP) neural network was explored [32] using satellite-based Aerosol Optical Depth (AOD), meteorological data and past PM2.5 data. The optimized version of the BP network using a genetic algorithm is proposed in [33].

Few researchers have also explored the hybrid model approach for prediction. A hybrid approach based on the autoregressive and nonlinear model for prediction of NO2 is proposed in [34]. A hybrid approach based on Autoregressive Integrated Moving Average Model (ARIMA) and ANN is discussed in [35]. The Comprehensive Forecasting Model (CFM) was developed based on ARIMA, ANN and Exponential Smoothing Method (ESM) [36]. Another cluster-based hybrid approach using Neural Network Autoregression (NNAR) and the ARIMA model is discussed in [37] for prediction of PM2.5 using past data of PM2.5. A hybrid-generalized autoregressive conditional heteroskedasticity based prediction approach proposed in [38] for prediction of PM2.5. In [39] hybrid model was built for PM2.5 by applying the trajectory-based geographic model and wavelet transformation into the MLP type of neural network. In which meteorological forecasts and pollutants were used as predictors. Comparison of a hybrid model consisting of an Ensemble Empirical Mode Decomposition and General Regression Neural Network (EEMD-GRNN), Adaptive Neuro-Fuzzy Inference System (ANFIS), Principal Component Regression (PCR), and MLR is discussed in [40] with best results obtained for EEMD-GRNN model. In [41] multi-task learning framework is used for the prediction of air pollutants which reduces model parameters with improved performance. Convolutional generalization model implemented [42] for prediction of PM2.5 using meteorological data shows MSE of 15.0 µg/m³. A deep learning-based prediction approach is also implemented for prediction using current and/or previous air pollutants and meteorological data [43–45].

The research work in [46] focused on Cuckoo Search-Least Squares Support Vector Machine (CS-LSSVM) based prediction approach for PM2.5 using correlation and principal component analysis. Previous data of PM2.5 was used as one of the predictors in addition to correlated parameters. The correlation analysis of PM2.5 to other meteorological parameters and pollutants using multivariate statistical analysis method and ANN was implemented in [47] and prediction results show RMSE of 24.06 µg/m³ for ANN-based model. Performance comparison of machine learning approaches such as Random Forests (RF), Support Vector Machines (SVMs) and ANN is presented in [48]. Furthermore, a calibration model is developed using ANN for black carbon in which meteorological parameter and other correlated pollutants are used as predictors. The lower RMSE and R² closeness to 1, also showed the effectiveness of the ANN.

However, the previously developed prediction model based on past data of predictand does not eliminate the need for dedicated instruments and in almost all cases the proprietary tools are used to measure the predictand. This presents an opportunity for developing a prediction model in the form of analytical equations based on the correlation. The ANN is adopted in our work, due to its superior performance discussed in [24, 30, 48]. Primary results related to the comparison of SVM and ANN are discussed in the results section and demonstrate the effectiveness of our proposed method.

The contribution of the work is as follows:

1. The study related to correlation of the pollutants with PM2.5 and additionally the correlation among the pollutants is performed for deciding the predictors.
2. Analytical equations are proposed for prediction of PM2.5 using ANN.
3. Recalibration of the derived prediction model in terms of coefficients and number of predictors is done to evaluate its performance.
3 Introduction to ANN Model

The proposed prediction model to obtain PM2.5 is based on supervised machine learning. It consists of interconnected computing elements known as neurons with inputs and outputs. As shown in Fig. 1, the model of a neuron has \(P\) inputs each with weight \(W\). The sum \((S)\) of weighted inputs and bias \((b)\) is fed to the transfer function block \((f)\). The output of each neuron is obtained by subsequently applying the transfer function to the sum of weighted inputs and bias.

The proposed PM2.5 prediction model using the ANN is derived using the following steps.

I Collection of large input data (observations) set for different pollutants.
II Preprocessing of the input data set to remove outliers.
III Finding correlation of PM2.5 with other pollutants using preprocessed input data set.
IV Based on the correlation results selection of input pollutants (predictors) for developing the prediction model of PM2.5.
V Selection of ANN topology for developing the prediction model.
VI Division of predictors data set into two sets, SET1: 90\% of data set or developing model (training, validation, and testing), SET2: 10\% of data set as unseen data set for further testing.
VII Developing 100 different ANNs with randomly initialized weights and biases using SET1.
VIII Testing of 100 different ANNs using SET2.
IX Based on performance indices selection of best ANN for the prediction model.
X Deriving analytical equation for prediction using selected ANN.
XI Prediction of PM2.5 using derived analytical prediction equation.

4 Observed Data and Correlation

To select the inputs for the PM2.5 prediction model, it is necessary to obtain the correlation between PM2.5 and pollutants besides the correlation among the pollutants. In the proposed study, Step I is the data collection phase: In this phase, 13 different parameters (pollutants and meteorological parameters) were collected from a CPCB online station, India (N 23° 0' 16.6287, E 72° 35' 48.7816). The data is collected for 41 months, where, the samples of data are taken every hour. Thirteen different parameters monitored from this online station includes pollutants; CO, NO, NO\(_2\), SO\(_2\), O\(_3\), VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene), PM2.5 and meteorological parameters; temperature and humidity. Dataset obtained from CPCB online station for all 13 parameters was containing a total of 29,928 observations. Due to maintenance, all the parameters data were not available simultaneously for 29,928 observations. After removing maintenance data for each of the parameters, 18,880 observations data set was available simultaneously for all 13 parameters. These 18,880 observations data set was smoothed out to remove the outliers [Step II] and is treated as the golden standard data. The smoothing of the data is done by a moving average filter, which was implemented in MATLAB. The optimum window size for smoothing was found to be 500, resulting in reasonably smoothed data. After smoothing, the first 500 results were removed, as the window size was 500. So, smoothed data of size 18,380 was used for developing the prediction model. Fig. 3 to Fig. 6 shows the original and smoothed data for all 13 parameters.
Correlation between any two parameters $x$ and $y$ is expressed by the correlation coefficient $R$ as per Eq. (1).

$$R = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{n \sum x^2 - (\sum x)^2} \ast (n \sum y^2 - (\sum y)^2)}$$

(1)

where $n$ is the total number of samples. $R$ takes values in the range of [-1 to +1]. For a strong positive correlation between $x$ and $y$, the value of $R$ will be close to +1 and vice-versa. For the practical purpose, correlation greater than 0.8 is assumed as being strong and less than 0.5 as weak [50].

### Table 1 Correlation among the Different Parameters

|       | CO    | NO    | NO₂   | SO₂   | O₃    | T     | RH    | Ben   | Tol   | Eth   | M-xyl | O-xyl | PM2.5 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| CO    | 1     | 0.936 | 0.872 | 0.828 | 0.771 | -0.069| -0.215| 0.901 | 0.927 | 0.909 | 0.909 | 0.909 | 0.830 |
| NO    | 0.936 | 1     | 0.927 | 0.826 | 0.789 | -0.122| -0.230| 0.927 | 0.927 | 0.909 | 0.907 | 0.860 | 0.909 |
| NO₂   | 0.872 | 0.927 | 1     | 0.728 | -0.075| -0.313| 0.919 | 0.849 | 0.828 | 0.809 | 0.769 | 0.909 | 0.845 |
| SO₂   | 0.828 | 0.826 | 0.927 | 1     | 0.714 | -0.099| -0.328| 0.881 | 0.817 | 0.790 | 0.766 | 0.769 | 0.845 |
| O₃    | 0.771 | 0.789 | 0.728 | 1     | 0.714 | -0.099| -0.328| 0.881 | 0.817 | 0.790 | 0.766 | 0.769 | 0.845 |
| T     | -0.069| -0.122| -0.198| -0.089| -0.066| 1     | 0.241 | -0.120| -0.158| -0.101| -0.219| -0.129| -0.180|
| RH    | -0.215| -0.230| -0.313| -0.328| -0.238| 0.294 | 1     | -0.318| -0.297| -0.323| -0.315| -0.324| -0.222|
| Benzene | 0.901 | 0.927 | 0.919 | 0.881 | 0.844 | -0.126| -0.318| 1     | 0.956 | 0.943 | 0.934 | 0.891 | 0.919 |
| Toluene | 0.928 | 0.927 | 0.849 | 0.817 | 0.849 | -0.158| -0.297| 0.956 | 1     | 0.989 | 0.982 | 0.955 | 0.877 |
| Ethyl benzene | 0.908 | 0.909 | 0.828 | 0.790 | 0.849 | -0.191| -0.323| 0.943 | 0.989 | 1     | 0.989 | 0.963 | 0.880 |
| M-P Xylene | 0.921 | 0.907 | 0.809 | 0.766 | 0.833 | -0.217| -0.315| 0.934 | 0.962 | 0.989 | 1     | 0.964 | 0.855 |
| O-Xylene | 0.894 | 0.860 | 0.769 | 0.769 | 0.833 | -0.127| -0.324| 0.891 | 0.955 | 0.963 | 0.964 | 1     | 0.818 |
| PM2.5 | 0.830 | 0.909 | 0.909 | 0.845 | 0.773 | -0.080| -0.222| 0.919 | 0.877 | 0.880 | 0.855 | 0.818 | 1     |

**Fig. 3** Original and Smoothed Data of CO, NO and NO₂ and SO₂.
Fig. 4 Original and Smoothed Data of O₃, Temperature, Humidity and Benzene

Fig. 5 Original and Smoothed Data of Toluene, Ethyl Benzene, M-P Xylene and O-Xylene
Correlation between PM2.5 and other parameters in addition to the correlation among the parameters is evaluated [Step III] based on the 18k+ data over a period of 41 months. The obtained results are shown in Table 1. As can be seen, the highest correlation of PM2.5 is found with NO, NO\textsubscript{2} and Benzene and low correlation with temperature and humidity. At typical ambient concentrations, NO is not considered to be hazardous while NO\textsubscript{2} can be hazardous [51]. Furthermore, NO\textsubscript{2} is considered as one of the major pollutants by world health organizations and environmental agencies [52,53]. Hence, NO\textsubscript{2} is considered as one of the predictors for the proposed model and NO is excluded. A strong correlation (>0.8) of CO, NO\textsubscript{2}, SO\textsubscript{2}, and VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene) with PM2.5 is observed which is useful in selecting the inputs for the PM2.5 prediction model.

The proposed prediction model is based on supervised learning, where, both inputs and target values are provided as a training dataset. So, for the proposed PM2.5 prediction model, as a training dataset, values of input pollutants (CO, NO\textsubscript{2}, SO\textsubscript{2}, and VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene)) and target (PM2.5) are taken. It is observed that the training of the ANN will be efficient if each parameter of the training dataset is normalized within the range [-1:1]. Normalization of the parameters is done by finding the value of each parameter within the normalized range using Eq. (2).

\[
x_n = \frac{(Y_{\text{max}} - Y_{\text{min}}) \cdot (X - X_{\text{min}})}{(X_{\text{max}} - X_{\text{min}})} + Y_{\text{min}}
\]

(2)

where \(X\) is the value of the parameter while \(X_{\text{max}}\) and \(X_{\text{min}}\) are the maximum and minimum values of the parameter, respectively. For example, in CO data, \(X\) is the smoothed value of CO while \(X_{\text{max}}\) and \(X_{\text{min}}\) are maximum and minimum values of smoothed CO data, respectively. As normalization range is [-1:1], \(Y_{\text{max}}\) is 1 and \(Y_{\text{min}}\) is -1. The normalized parameters can be converted back into their original form using Eq. (3).

\[
x = \frac{(x_n - Y_{\text{min}}) \cdot (X_{\text{max}} - X_{\text{min}})}{(Y_{\text{max}} - Y_{\text{min}})} + X_{\text{min}}
\]

(3)

where \(x_n\) represents normalized data and \(X\) is the smoothed data. \(X_{\text{max}}\) and \(X_{\text{min}}\) are the maximum and minimum values of smoothed data, respectively. For example, to convert the normalized data of predictand PM2.5 into original form, \(X_{\text{max}}\) and \(X_{\text{min}}\) values of targeted PM2.5, shown in Fig. 6 are used.

5 Prediction model of PM2.5

In the proposed prediction model (see Fig. 7), inputs are selected based on the correlation results [Step IV]. As can be seen from Table 1 a higher correlation (>0.8) of CO, NO\textsubscript{2}, SO\textsubscript{2}, and VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene) with PM2.5 is observed. So, out of 12 parameters 8 parameters; CO, NO\textsubscript{2}, SO\textsubscript{2}, and VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene) are selected for developing the PM2.5 prediction model. Additionally, as the number of input parameters is reduced from 12 to 8, the computation cost of the proposed...
The prediction model of PM2.5 shown in Fig. 7 is based on a feed-forward neural network with a single hidden layer [Step V]. Selected eight pollutants are the input parameters for each neuron of the hidden layer which consists of eight neurons.

The weights of the hidden layer and output layer can be represented by a matrix of size $S \times P$, where, $S$ is equal to the number of neurons in the layer and $P$ is equal to the number of inputs of the layer. In our case, the matrix size is $8 \times 8$, as both the inputs and hidden layer size are 8. The matrix size for the output layer is $1 \times 8$ as it consists of one neuron and eight inputs coming from the hidden layer. For the proposed predicted model, weights of the hidden layer and output layer are represented by $LW_1$ of $(8 \times 8)$ size and $LW_2$ of size $(1 \times 8)$ respectively.

The training function $\text{trainlm}$ based on the Levenberg-Marquardt algorithm is adopted [54, 55] for training. To train the network for the nonlinear relationship between input and output and to constrain output in positive range standard nonlinear transfer function $\text{logsig}$ given by Eq. (4) is used in the hidden layer.

$$\text{logsig}(m) = \frac{1}{1 + e^{-m}}$$

where $m$ is the input to the transfer function. In $\text{logsig}$ transfer function, the output will be in the range of [0:1] for the entire range of inputs. For nonlinear regression or prediction, $\text{purelin}$ is an effective transfer function for the output layer [56]. Hence in the proposed model, $\text{purelin}$ is used as a transfer function in the output layer. In $\text{purelin}$, the output will be equal to the input.

The total available data of 18k+ is divided into two sets the first set (SET1) includes 90% of data and the second set (SET2) includes 10% of data [Step VI]. The division into two sets is done randomly so that all types of data can be included in two sets. The SET1 (90% data) is used for designing the neural network and it is divided in a standard manner widely used by researchers, 70% for training, 15% for validating and 15% for testing. The SET2 (10% data) is kept as unseen data for further testing and comparing the performance of neural networks.

For selecting the best ANN for prediction model, 100 different ANNs are developed and tested as per the pseudo-code in Algorithm 1 This algorithm is repeated 100 times to get the performance of 100 different ANNs for comparing training and testing results with good generalization [Step VII, VIII]. The performance of the ANN is

![Fig. 7 Selected ANN Topology for Prediction](image-url)
Algorithm 1: Pseudo Code for Developing and Testing 100 different ANNs

1: Load the data SET1 for developing the network and SET2 to test the Network for unseen data
2: for i = 1 to 100 do
3:   Divide SET1 randomly for training(70%), validating(15%) and testing (15%)
4:   Initialize the weights and biases
5:   Train the network
6:   Validate the network
7:   Test the network
8:   Evaluate training, validation and testing performance
9:   Save the performance results
10:  Save Network and its weights and biases
11:  Test the Network performance for unseen data using SET2
12:  Save the performance results
13:  end for

evaluated [Step IX] based on, RMSE and R², where, RMSE is the root mean square of the errors, i.e, the difference between the target value and the predicted value and is given in Eq. (5).

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{n}(A_i - P_i)^2}{n}}
\]  

(5)

where \(A_i\) represents the actual value, \(P_i\) represents the predicted value and \(n\) is the total number of samples. \(R^2\) is the coefficient of determination and it is the square of the correlation \(R\) (Eq. (1)). The closeness between target values and predicted outputs of ANN is represented by \(R^2\). The value of \(R^2\) equal to 1 represents targets and predicted outputs are very close to each other.

5.0.1 Model Equations

The hidden layer and output layer weights for the proposed model are shown in Eq. (6) and Eq. (7) respectively. The biases of the model for hidden layer and output layer are shown in Eq. (8) and Eq. (9) respectively. Matrix \(B_1\) is formed by repeating the hidden layer bias matrix \(b_1\), \(N\) times, where \(N\) is equal to the size of test dataset (1838 in our case). This operation shown in Eq. (10), is performed to make bias matrix size \(B_1\) equal to the size of product term matrix \(LW_1 \times x_n\), so that addition operation \((B_1 + LW_1 \times x_n)\), shown in Eq. (11) can be performed.

\[
LW_1 = \begin{bmatrix}
-25.978 & -31.063 & 17.505 & 38.446 & -37.353 & 97.708 & -92.951 & 65.964 \\
3.295 & 6.460 & 0.203 & -1.981 & 10.078 & -10.281 & 3.352 & -3.782 \\
-2.661 & 2.503 & -1.075 & -1.011 & -0.194 & 1.702 & -2.768 & 1.690 \\
-6.069 & 6.142 & -2.212 & -3.593 & 1.800 & -3.002 & 0.222 & 2.803 \\
-9.788 & -7.748 & -4.424 & 27.227 & -4.406 & 0.016 & -6.279 & 8.460 \\
3.821 & -6.233 & 1.243 & -1.449 & 5.600 & 1.846 & 1.801 & -5.862 \\
3.149 & 6.319 & 0.368 & -0.825 & 10.746 & -11.220 & 2.650 & -3.428 \\
-2.127 & 1.991 & -1.116 & -0.032 & 0.038 & 4.094 & -4.882 & 1.330
\end{bmatrix}
\]  

(6)

\[
LW_2 = \begin{bmatrix}
0.158 & -17.591 & -6.481 & 1.614 & -0.369 & -0.817 & 17.345 & 4.950
\end{bmatrix}
\]  

(7)

\[
b_1 = \begin{bmatrix}
34.474 \\
4.001 \\
-1.015 \\
-2.615 \\
5.700 \\
-0.148 \\
4.383 \\
-1.959
\end{bmatrix}
\]  

(8)

\[
b_2 = \begin{bmatrix}
1.593
\end{bmatrix}
\]  

(9)

\[
B_1 = [b_1 \ b_1 \ b_1 \ \ldots \ \ldots \ \ldots N]
\]  

(10)
The prediction model for deriving PM2.5 [Step X] is given by Eq. (11).

\[
PM_{2.5n} = b_2 + LW_2 \times \text{logsig}(B_1 + LW_1 \times x_n) \tag{11}
\]

where \(PM_{2.5n}\) is normalized output. The input matrix \(x_n\) is formed using normalized values of CO, NO\(_2\), SO\(_2\), and VOC and the size of \(x_n\) is \(P \times N\) where \(P=8\) is the number of inputs and \(N=1838\) is the number of values for each input. Eq. (11) shows the usefulness of the approach to obtain the value of PM2.5 based on CO, NO\(_2\), SO\(_2\), and VOC values only. Therefore, low-cost sensors can be deployed with the derived model that offers the opportunity to derive PM2.5 through signal processing algorithms. Eq. (12) shows the conversion to the original value from the normalized one using Eq. (3), in which \(X_{\text{max}}\) and \(X_{\text{min}}\) are taken as per Fig. 6.

\[
PM_{2.5} = \frac{(PM_{2.5n} + 1) \times (180.052 - 2.228)}{2} + 2.228 \tag{12}
\]

The proposed approach based on the above analytical equations eliminates the need for proprietary tools. The analytical equation for the prediction can be computed using any low-cost processing tool (e.g., excel sheet etc.). A screenshot of an example [Step XI] is shown in Fig. 8. In this example, an input matrix \(x\) of size \(8 \times 1838\) is taken which represents the testing data set. Eq. (11) is computed as follows.

a. First, \(x_n\) is obtained by computing Eq. (2).
b. Multiplying the two matrices of \(LW_1\) (Eq. (6)) and \(x_n\), product term \(LW_1 \times x_n\) is obtained.
c. Matrix \(B_1\), formed using Eq. (10) is added in the product term \(LW_1 \times x_n\).
d. Hidden layer activation function (Eq. (4)) is applied to find the output of the hidden layer.
e. The output of the hidden layer is multiplied by \(LW_2\) (Eq. (7)).
f. Then matrix \(b_2\) from Eq. (9), is added.

Finally, \(PM_{2.5n}\) (marked as \(A\) in Fig. 8) is obtained by computing Eq. (11), which is the normalized value of PM2.5. PM2.5 in the original unit is obtained by processing Eq. (12) (marked as \(B\) in Fig. 8). Predicted values of PM2.5 obtained from Eq. (12) (marked as \(B\) in Fig. 8) are close to the actual values of PM2.5 (marked as \(C\) in Fig. 8). Interestingly these computations can be ported to a wireless sensor node having basic memory along with computational capability and the algorithms can still perform reliably.

![Fig. 8 Excel sheet used for processing prediction model equation](image-url)

The deployment of the developed prediction model needs to consider the following limitations based on the location, available monitoring stations and available monitoring parameters as predictors.

- Air pollution varies from one location to another based on the few parameters like human activity, traffic condition, the structure of urban area and weather conditions. Based on the location, predictors and predictand values as well as their maximum and the minimum limit will change. So, the application of the presented
prediction model for another location needs model training, validation, and testing again which provides new coefficients in terms of weights and biases for accurate prediction with lower RMSE.

• Application of prediction model to another location requires a large set of authentic data for training which is sometimes difficult due to the limitation on the number of online environment monitoring stations. Due to a few monitoring parameters, and delay in the availability of data; offline stations are less preferable than online stations.

• Online stations of CPCB monitors pollutants that are greater than the offline stations. Concentration data for a large set of pollutants is the basic requirement for a correlation study or developing a prediction model. Due to the limitation on the online stations available in the city, data were used from only one online station for training, validation, and testing in the proposed study. This can be expanded in the future by taking data from multiple online stations of different cities.

• The derived prediction model based on ANN generally shows poor performance for predicting the sudden large change in predictors. As, sometimes it is difficult to discriminate between the outliers and sudden change in the value, applying a smoothing algorithm to remove outliers will also remove the sudden large change in the value of the predictor. This limitation can be targeted through different data processing algorithm and is left as part of future work.

5.0.2 Model Results

In comparison to Support Vector Machine (SVM), the ANN exhibits better performance in terms of RMSE. The RMSE of 2.862 and 2.823 is obtained during training and testing respectively for the SVM model (shown in Table 2). While for ANN, the RMSE of 1.5971 and 1.5121 is obtained (shown in Table 3) during training and testing for unseen data respectively.

Table 3 shows the best performance of the prediction model obtained from 100 iterations. The value of \( R^2 \) demonstrates the closeness of the predicted values with the target values or actual values. The actual values of PM2.5 are compared (see Fig. 9) with predicted results obtained by Eq. (12). It is found that the predicted results are in close accordance with actual values, which confirms the effectiveness of the proposed approach.

**Table 2 Performance of SVM**

| Performance of | RMSE |
|---------------|------|
| Training      | 2.862|
| Testing for unseen data | 2.823|
Table 3 Performance of Prediction Model

| Performance of | RMSE  | R²   |
|---------------|-------|------|
| Training      | 1.5971| 0.9987|
| Validation    | 1.6347| 0.9986|
| Testing       | 1.5843| 0.9988|
| Testing for unseen data | 1.5121| 0.9988|

Table 4 Summary of previously developed prediction models

| Reference | Predictand | RMSE  | R²   |
|-----------|------------|-------|------|
| [25]      | O₃ (ppb)   | 0.30  | 0.69 |
| [26]      | O₃ (µg/m³) | 21.78 | 0.73 |
| [27]      | NO₂ (ppb)  | 7.3   | 0.91 |
| [34]      | NO₂ (µg/m³) | 13.93 | 0.93 |
| [28]      | PM 10 (µg/m³) | 12.16 | 0.83 |
| [35]      | PM 10 (µg/m³) | 11.656 | 0.983 |
| [32]      | PM2.5 (µg/m³) | 12.8935 | - |
| [34]      | PM2.5 (µg/m³) | 12.7 | 0.954 |
| [29]      | PM2.5 (µg/m³) | 6.77 | 0.99 |
| [40]      | PM2.5 (µg/m³) | 5.0324 | 0.79 |
| [49]      | PM2.5 (µg/m³) | 14.47 | - |
| [47]      | PM2.5 (µg/m³) | 21.06 | - |
| [48]      | BC (ng/m³) | 1480.746 | 0.586 |
| This Work | PM2.5 (µg/m³) | 1.7973 | 0.9986 |

Previously developed prediction models, depend on past data, are often time-consuming and use dedicated instruments. In the prediction model, we have eliminated the above requirements and comparison with some researches is shown in Table 4. As can be seen, the proposed approach has better RMSE and R² compared to existing methods. The RMSE of 1.7973 µg/m³ and R² of 0.9986 is obtained for test dataset of size 1838. We extended the model to accommodate a reduced test dataset of size 10, which shows RMSE of 146.10 µg/m³ and R² of 0.9467. The proposed model in the form of the analytical equation thus helps in predicting PM2.5 using low-cost processing tools or existing WSN.

The proposed prediction model is recalibrated in terms of the number of predictors, weights, and biases to show the effectiveness of the proposed approach. Instead of eight predictors, three predictors, CO, NO₂, and Benzene (VOC component) are taken considering the availability of low-cost sensors [57] which includes this type of multiple sensing parameters. The proposed approach can work for any other three sensing parameters after recalibrating model. In recalibration, CPCB smoothed data for CO, NO₂, and Benzene (VOC component) are used as it is considered as golden standard data. For recalibration ANN shown in Fig. 7 is used with the same training and testing dataset (of three parameters), but the size of the input layer and the hidden layer is reduced to three. Extracted weights and biases are represented in Eq. (13) to Eq. (16). Performance results are shown in Table 5. Results show, during testing RMSE is 7.5372 µg/m³ and R² is 0.9708.

\[
WL_1 = \begin{bmatrix} 26.281 & 3.456 & -12.391 \\ 17.898 & -0.863 & 11.305 \\ -0.996 & -0.502 & -1.205 \end{bmatrix} \quad (13)
\]

\[
WL_2 = \begin{bmatrix} -1.008 & 1.379 & -1.665 \end{bmatrix} \quad (14)
\]

\[
b_1 = \begin{bmatrix} 9.934 \\ 21.939 \\ 1.101 \end{bmatrix} \quad (15)
\]

\[
b_2 = [0.689] \quad (16)
\]
Table 5: Performance of Prediction Model for Three Predictors

|                | RMSE (µg/m³) | R²  |
|----------------|--------------|-----|
| Training       | 7.9297       | 0.9678 |
| Validation     | 8.0954       | 0.9679 |
| Testing        | 8.0649       | 0.9672 |
| Testing for unseen data | 7.5372 | 0.9708 |

6 Conclusion and Future Work

In this work, we have studied the correlation of PM2.5 with other pollutants and correlation among the pollutants, based on the standardized CPCB data. The prediction model of PM2.5 is based on the correlation and shown to be useful for online as well as offline measurements. The proposed model is in the form of analytical equations that enables the use of any low-cost processing tool and eliminates the need for a proprietary tool for predicting PM2.5 values. Results obtained using this method with eight predictors (NO₂, SO₂, and VOC (Benzene, Toluene, Ethyl Benzene, M+P Xylene, O-Xylene)) shows RMSE of 1.7973 µg/m³ and R² of 0.9986 for the test dataset. To show the effectiveness of the proposed approach, the derived prediction model was recalibrated with three predictors (CO, NO₂, and Benzene (VOC component)) due to the possibility of sensing all three parameters by one or two low-cost sensors. The proposed approach can work for any other three sensing parameters too after recalibration. Testing results show RMSE of 7.5372 µg/m³ and R² of 0.9708. The obtained results prove the effectiveness of the proposed approach. The obtained results can be improved in the future by recalibrating prediction model based on the data available from multiple stations located at the place of deployment. In comparison to existing methods, the proposed approach facilitates an efficient method that reduces overall computation cost. Furthermore, this model can be implemented on the wireless sensor node for automated measurement of PM2.5.

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Compliance with ethical standards

Conflict of interest: The authors declare that they have no conflict of interest.

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